

The $1/N$ expansion in quantum mechanics

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We consider the application of the $1/N$ expansion to the calculation of energies (of both discrete levels and quasi-stationary states) and wave functions, as well as to the problem of two Coulomb centers and the three-body problem. We show that in many cases (for example, for the $c\bar{c}$ charmonium states) the method yields high accuracy even for low quantum numbers, including the ground state. The relation of these results to the properties of minimizing-uncertainty coherent states is discussed.

1. INTRODUCTION

At the present time the $1/N$ expansion is widely used in quantum mechanics and field theory (see, e.g., Refs. 1–16). The procedure consists in first generalizing to a space of arbitrary dimension D and then taking the limit as $D \rightarrow \infty$, which is equivalent in quantum mechanics to $\hbar \rightarrow 0$ or $M \rightarrow \infty$. In that limit the problem reduces to the classical motion of the particles and, in particular, to the determination of the equilibrium orbit or (in the case of several particles) the equilibrium classical configuration. Taking into account the effect of quantum fluctuations about it and effects of anharmonicity leads to the expansion

$$E_{nl} = E_{nl}^{(0)} + E_{nl}^{(1)} N^{-1} + E_{nl}^{(2)} N^{-2} + \dots, \quad (1.1)$$

whose coefficients can be calculated recursively. The physical dimension $D = 3$ is then substituted in the final formulas resulting in a good approximation to the exact solution.¹⁾

Different versions of this method result from different choices of the expansion parameter: $N = 1 + D/2$, where $l = 0, 1, \dots$ is the orbital angular momentum; $N = l + \frac{1}{2}D$ —a (“shifted” $1/N$ expansion^{5,9}); $N = [l(l+1)]^{1/2}$ for $D = 3$ (see Ref. 16). The $1/N$ expansion has been worked out in greatest detail for problems with spherical^{2,5–10} and axial symmetry (hydrogen atom in magnetic⁴ and electric^{13,14} fields). In Refs. 10 and 11 the $1/N$ expansion was considered for the three-body problem.

Usually the $1/N$ expansion is applied to the discrete spectrum. In Ref. 12 it was shown how to apply it to obtain the energies and widths ($E = E_r - i\Gamma/2$) of resonant states. This made possible the utilization of this method in the theory of the Stark effect in a strong field,^{13,14} which turned out to be particularly convenient in the case of Rydberg states.

The present paper is devoted to the following questions: 1) application of the $1/N$ expansion to the calculation of energies and wave functions; 2) precision of the method in the case of low quantum numbers; 3) application to the problem of two Coulomb centers and to the three-body problem; 4) the $1/N$ expansion and coherent states.

2. ENERGY CALCULATION

We consider the attractive potential

$$V(r) = -(\hbar^2/MR^2)gv(x), \quad x = r/R, \quad (2.1)$$

(g is a dimensionless coupling constant, $n = p + l + 1$, $p = 0, 1, \dots$ is the radial quantum number (often denoted by n_r), l is the orbital angular momentum;

from now on $\hbar = M = 1$). If $n \rightarrow \infty$ while p is fixed then the particle is localized near the classical equilibrium point $x = x_0$, determined by the equation¹²

$$x^3 v'(x) = -v, \quad (2.2)$$

where $v = n^2 g^{-1}$, the energy $E_{nl} = (g^2/2n^2 R^2) \epsilon_{nl}$ and

$$\epsilon = \epsilon^{(0)} + \epsilon^{(1)}/n + \epsilon^{(2)}/n^2 + \dots \quad (2.3)$$

Thus we have $D = 3$, $l \rightarrow \infty$, and $N \equiv n$ (in the case of the Coulomb field n coincides with the principal quantum number of the level) so that in the following we shall speak of the $1/n$ expansion.

Comparison of the Schrödinger equation for $r \sim r_0 = Rx_0$ with the equation for the harmonic oscillator shows that the role of the parameter n is played by the ratio M/\hbar . The amplitude of the zero-point vibrations of the oscillator is proportional to $(\hbar/M\omega)^{1/2} \propto n^{-1/2}$ so that we put accordingly

$$x = x_0(1 + \xi n^{-1/2}) \quad (2.4)$$

and expand the quantities entering the Schrödinger equation in powers of $n^{-1/2}$ (in contrast to r , the variable ξ remains finite in the limit as $n \rightarrow \infty$). In this way we determine successively the coefficients in Eq. (2.3) and the corresponding coefficients (in powers of $n^{-1/2}$) for the wave functions. For example:

$$\begin{aligned} \epsilon^{(0)} &= (1+v_0)v^2/x_0^2, \quad \epsilon^{(1)} = (2p+1)(\omega-1)v^2/x_0^2, \\ \epsilon^{(2)} &= (v/\omega^2 x_0^2)^2 \{ \frac{3}{2}(2p+1)^2 \omega(\sigma-\omega^2) \\ &+ \frac{1}{2} \omega^2(\tau+1) - \frac{11}{16} \sigma^2 + p(p+1)[\omega^4 + \omega^2(\tau-1) - \frac{15}{8} \sigma^2] \}, \end{aligned} \quad (2.5)$$

where we have introduced the following notation:

$$\omega = [3(1+v_2)]^{1/2}, \quad \sigma = 4(1-v_3), \quad \tau = \frac{15}{2}(v_4 + \frac{3}{5}), \quad (2.6)$$

$$v_k = \frac{2}{(k+1)!} x^{k-1} \frac{d^k v}{dx^k} \bigg|_{x=x_0} \quad (2.7)$$

(we note that ω is the frequency of small vibrations about the equilibrium point x_0).

Analytic expressions for the coefficients $\epsilon^{(k)}$ that follow are quite unwieldy, however they are easily calculated with the help of recurrence relations¹⁶ convenient for computer calculations.

The case $E = 0$ (i.e., the instant of appearance of the bound state in the short-range potential) requires special

discussion. The "reduced" energy $\varepsilon(\nu)$, as a rule, increases with increasing ν and for some $\nu = (\nu_{cr})_{nl}$ the level is expelled into the continuum. In the zeroth approximation ($n \rightarrow \infty$) we have

$$\nu_{cr} = 2\bar{x}_0^2 v(\bar{x}_0), \quad \left. \frac{d\varepsilon^{(0)}}{d\nu} \right|_{\nu=\nu_{cr}} = 2v(\bar{x}_0), \quad (2.8)$$

where \bar{x}_0 is the root of the equation $xv' + 2v = 0$. Order $1/n$ corrections may be obtained from Eqs. (2.3) and (2.5). Denoting by g_{nl} the coupling constant corresponding to zero energy of the nl -level we have

$$g_{nl} = \frac{n^2}{2\bar{x}_0^2 v(\bar{x}_0)} \left[1 + \frac{\alpha_1}{n} + \frac{\alpha^2}{n^2} + O\left(\frac{1}{n^3}\right) \right], \quad (2.9)$$

$$\alpha_1 = (2p+1)(\omega-1),$$

$$\alpha_2 = \frac{1}{2} [\omega^2 - \omega - 5 + (3\sigma + \tau + 3)/\omega^2 - 11\sigma^2/8\omega^4] + p(p+1) [2\omega^2 - 2\omega - 9 + (6\sigma + \tau + 3)/\omega^2 - 15\sigma^2/8\omega^4], \quad (2.10)$$

(we take ω , σ , and τ at $x = \bar{x}_0$).

With further increase of the parameter ν (for $\nu = \nu_* > \nu_{cr}$) the frequency ω may become vanishing. At that point the classical solution becomes unstable—a collision occurs between the two solutions corresponding to stable and unstable equilibrium points in the effective potential $U(r)$, which includes the centrifugal energy. For $\nu > \nu_*$ $U(r)$ no longer has a minimum for real $0 < r < \infty$, the equilibrium point $x_0(\nu)$ moves off into the complex plane, and the coefficients in the $1/n$ expansion become complex. Such a solution, making no physical sense from the point of view of classical mechanics, is of particular interest on going over to quantum mechanics: it is precisely the solution that defines within the framework of the $1/n$ expansion not just the location but also the width of the resonant states. For further details see Refs. 12 and 17.

3. THE WAVE FUNCTIONS AND $\psi(0)$

The calculation of the wave functions (in particular, of the asymptotic coefficients for $r \rightarrow 0$ and $r \rightarrow \infty$) is of substantial interest.²⁾ By making use of just two terms of the $1/n$ expansion, analytic formulas asymptotically exact as $n \rightarrow \infty$ may be obtained for an arbitrary smooth potential $V(r)$.

To this end, having made the replacement (2.4), we note that in the region $|\xi| \ll n^{1/2}$ the function $\chi_{nl}(r) = rR_{nl}(r)$ coincides with the wave function of the p th level of the harmonic oscillator with frequency ω , Eq. (2.6). We continue it (with the help of the WKB method) into the subbarrier region $\xi < \xi_-$ or $\xi > \xi_+$, where $\xi_{\pm} = \pm [(2p+1)/\omega]^{1/2}$, and expand all quantities at the point $x = x_0$ in powers of $1/n$ thus obtaining the desired result. Here we shall list just the formula for the asymptotic coefficient at zero:

$$\chi_{nl}(r) = c_{nl} R^{-(l+1/2)} r^{l+1} + \dots, \quad r \rightarrow 0, \quad (3.1)$$

$$\tilde{c}_{nl} = \left[\frac{n\omega^3}{\pi(\rho!)^2} \right]^{1/4} (2\pi\omega)^{p/2} x_0^{p-1/2} \exp\{-[nJ_0 + (2p+1)J_1]\}, \quad (3.2)$$

(the tilde indicates that the expression is approximate),

$$J_0 = \ln x_0 + \int_0^{x_0} dx [Q_0(x) - x^{-1}], \quad (3.3)$$

$$J_1 = \frac{1}{2} \int_0^{x_0} dx \left[\frac{x_0}{x(x_0-x)} - \frac{P_0(x)}{Q_0(x)} \right],$$

where

$$Q_0(x) = \left[\frac{1}{x^2} - \frac{2}{\nu} v(x) - \frac{\varepsilon^{(0)}}{\nu^2} \right]^{1/4},$$

$$P_0(x) = x^{-2} + (\omega-1)x_0^{-2}.$$

Analogous expressions may be obtained for $r > r_+$, including that for the asymptotic coefficient for $r \rightarrow \infty$ and for the effective radius.²³⁾

The Eq. (3.2) retains its form also for the states with $E = 0$ provided one replaces x_0 by \bar{x}_0 [see Eq. (2.8)] and sets

$$P_0(x) = [1 + (\bar{\omega}-1)u]x^{-2}, \quad Q_0(x) = x^{-1}(1-u)^{1/4}, \quad (3.4)$$

where $\bar{\omega} = \omega(\bar{x}_0)$, $u = x^2 v(x) / \bar{x}_0^2 v(\bar{x}_0)$.

Lastly we consider the wave function for finite r , confining ourselves for simplicity to the nodeless states ($p = 0$, $n = l + 1$). Then

$$\chi_{n,n-1} = \left(\frac{n\omega}{\pi x_0^2} \right)^{1/4} \exp\left(-\frac{1}{2} \omega \xi^2\right) \times \left[1 + \left(\frac{1}{3} a \xi^3 + b \xi \right) n^{-1/2} + O(n^{-1}) \right], \quad (3.5)$$

where $a = 2(1 - v_3)\omega^{-1}$, $b = (a - 1)\omega^{-1}$ and

$$\int_0^{\infty} \chi^2 dx = 1$$

accurate to terms of order $1/n$. This formula is valid near the equilibrium point x_0 , including the turning points x_{\pm} . The terms proportional to $n^{-1/2}$ take into account corrections due to anharmonicity and substantially improve the agreement between the expression (3.5) and numerical calculations.²³⁾

4. ACCURACY OF THE $1/n$ EXPANSION

Our formulas are asymptotically exact for $l \rightarrow \infty$ and p fixed. However in physical applications one needs usually $n \sim 1$. To begin with, it is not clear whether the $1/n$ expansion could be useful for low quantum numbers. To answer this question we consider a few examples (see also Refs. 15 and 23).

a) For power-law potentials

$$V(r) = gr^N/N \quad (4.1)$$

we have

$$E_{nl}(g) \propto g^{2/(N+2)}, \quad c_{nl}(g) \propto g^{(1+\nu/2)/(N+2)}$$

(scaling), so that it suffices to put $g = 1$. In this case

$$v(x) = -\frac{x^N}{N}, \quad v_k = 2 \frac{(N-1)!}{(k+1)!(N-k)!}, \quad x_0 = n^{2/(N+2)}$$

and the energy has the expansion:

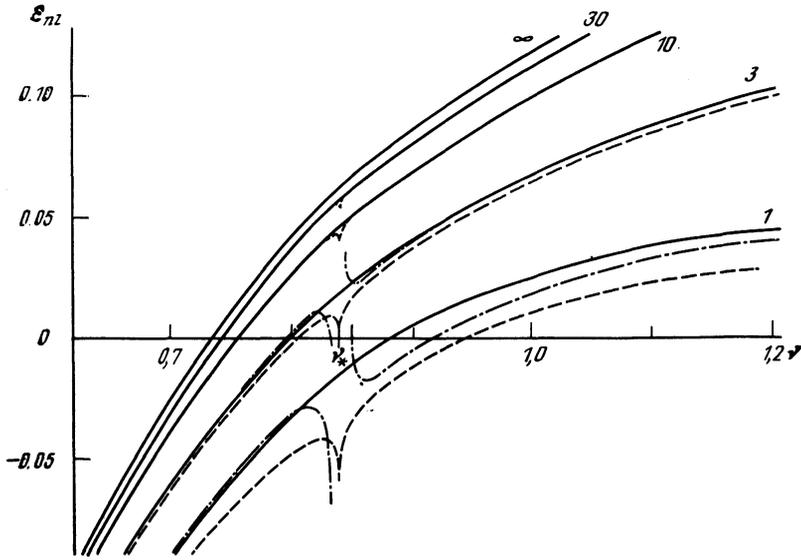


FIG. 1. Energies of the states with $l = n - 1$ in the Yukawa potential [for $\nu > (\nu_{cr})_{nl}$ we show $\text{Re } \epsilon_{nl}$]. The solid, dashed and dash-dot curves correspond to one, two, and three terms of the series (2.3). The curves are labeled by the l values.

$$E_{nl} = \frac{1}{2} n^2 N^{2(N+2)} (\alpha_0 + \alpha_1/n + \alpha_2/n^2 + \dots), \quad (4.2)$$

where

$$\begin{aligned} \alpha_0 &= 1 + 2N^{-1}, \quad \alpha_1 = (2p+1)(\omega-1), \\ \alpha_2 &= -[(N-2)/2(N+2)] [(2p+1)^2 \omega + 1/36(N^2 - 15N - 52) \\ &\quad + 1/6p(p+1)(N^2 - 9N - 34)], \end{aligned} \quad (4.3)$$

$\omega = (N+2)^{1/2}$. The coefficients α_k decrease rapidly with increasing k for $-1 \leq N \leq 4$. For $N = -1$ and 2 all $\alpha_k \equiv 0$ for $k \geq 2$ and the series (4.2) cuts off: $\epsilon_{nl} = -1$ for $N = -1$, $\epsilon_{nl} = 2n^3 [1 + (p+1/2)/n]$ for $N = 2$. The asymptote (3.2) is accurate to within one percent even for the ground state if $N \leq 6$ (for nodeless states).

b) For the description of quarkonium^{19,20} and multi-quark systems²¹ we use the funnel potential

$$V(r) = -\kappa/r + r/a^2, \quad (4.4)$$

for which

$$v(x) = x^{-1} - x, \quad R = (\kappa a^2)^{1/2}, \quad \omega = [(1+3x_0^2)/(1+x_0^2)]^{1/2},$$

with x_0 determined from the equation $x^3 + x = \nu \equiv n^2 \kappa^{-3/2} a^{-1}$. Hence

$$x_0 = 3^{-1/2} \{ [(1+t)^{1/2} + t^{1/2}]^{1/2} - [(1+t)^{1/2} - t^{1/2}]^{1/2} \}, \quad (4.5)$$

where $t = 6.75n^4 \kappa^{-3} a^{-2}$. Using Eq. (2.5) we find

$$\begin{aligned} \epsilon^{(0)} &= 3x_0^4 + 2x_0^2 - 1, \quad \epsilon^{(1)} = (2p+1)(1+x_0^2)^2(\omega-1), \\ \epsilon^{(2)} &= \frac{3}{2} \omega^{-4} [(2p+1)^2(1+x_0^2)^2 \omega - (1+3x_0^2 + 11/6 x_0^4) \\ &\quad - 4p(p+1)(1+19/6 x_0^2 + 7/4 x_0^4)]. \end{aligned} \quad (4.6)$$

Calculations using these formulas are elementary. A comparison with numerical calculations³⁾ is shown in Fig. 1, where the same values of κ and a were used as in the description of $c\bar{c}$ charmonium. Here one should keep in mind that scaling $r \rightarrow ar$ reduces the Schrödinger equation to the standard form

$$\frac{d^2 u_l}{d\rho^2} + \left(\xi + \frac{\lambda}{\rho} - \rho - \frac{l(l+1)}{\rho^2} \right) u_l = 0 \quad (4.7)$$

and the following relations hold between the parameters

$$\lambda = \kappa (2Ma)^{1/2}, \quad E_{nl} = (2Ma^4)^{-1/2} \xi_{nl}$$

Setting $2M = m_c = 1.84$ GeV, $\kappa = 0.52$ and $a = 2.34$ GeV⁻¹ (parameters of the Cornell potential²⁰) we obtain $\lambda = 1.37623$. As can be seen from Table I, the first three terms of the $1/n$ expansion determine the energy to an accuracy no worse than 1% and reproduce the charmonium spectrum quite well. It is noteworthy that using the formulas (2.5) one can easily perform the calculations for other potentials, arising in quantum chromodynamics, as well.

In Table I are also given values of the ratio \tilde{c}_{nl}/c_{nl} . The degree of agreement between the asymptote (3.2) and the exact coefficients c_{nl} for nodeless ($p = 0$) states is striking. However for $p \geq 1$ the agreement worsens, so that it becomes

TABLE I. Precision of the $1/n$ expansion for the funnel potential ($c\bar{c}$ charmonium).

State	$\xi_{nl}^{(l)}$		M , GeV			c_{nl} , Exact	\tilde{c}_{nl}/c_{nl}
	$1/n$	Exact	$1/n$	Exact	Exp.		
1S	0.9793 (0.1%)	0.980 366	3.097	3.097	3.097	2.0833	0.9977
1P	2.6114 (0.01%)	2.611 131	3.526	3.525	3.525	0.89695	0.9976
2S	3.2648 (1%)	3.228 853	3.697	3.688	3.686	1.6634	1.40
1D	3.6958 (0.005%)	3.695 599	3.811	3.810	3.770	0.31027	0.9983
2P	4.3027 (0.14%)	4.296 697	3.970	3.968	-	1.0701	1.22
3S	4.8944 (1.1%)	4.842 092	4.125	4.112	4.030	1.5362	-

desirable to include in (3.2) order $1/n$ correction (see Appendix 1).

c) For the Yukawa potential

$$v(x) = e^{-x} x^{-1}, \quad \omega = [1 - x_0^2 / (1 + x_0)]^{1/2}, \quad (4.8)$$

and the ν dependence of x_0 and $\varepsilon^{(0)}$ is determined parametrically.¹² In that case

$$\nu_{cr} = 2e^{-1} = 0.7358, \quad \nu_* = 0.8340. \quad (4.9)$$

As long as $\nu < \nu_*$, $x_0(\nu)$ and the coefficients $\varepsilon^{(k)}$ are real. For $\nu > \nu_*$ the coefficients in the $1/n$ expansion become singular

$$\varepsilon^{(0)} \propto (\nu_* - \nu)^{3/2}, \quad \varepsilon^{(1)} \propto (\nu_* - \nu)^{1/2}, \quad \varepsilon^{(2)} \propto (\nu_* - \nu)^{-1},$$

and $\varepsilon^{(k)} \rightarrow \infty$ starting with $k = 2$. Therefore the $1/n$ expansion is inapplicable near $\nu \approx \nu_*$, but for $\nu > \nu_*$ (when the equilibrium point $x_0(\nu)$ moves off into the complex plane) it again becomes applicable (see Fig. 1). Just as in the case of the funnel, three terms of the series (2.3) ensure good accuracy for the energy calculation, which only improves with increasing l .

d) The Tietz potential²⁶

$$V(r) = -1/r(1 + \mu r)^2 \quad (4.10)$$

is a good approximation to the Thomas-Fermi potential in neutral atoms and at the same time permits an analytic solution^{26,27} for $E = 0$. At the instant of appearance of the nl -level one has $(\mu_{cr})_{nl} = 2/(n+l)(n+l+1)$, which for the potential written in the form (2.1) gives

$$(g_{cr})_{nl} = 2n^2 \left[1 - \frac{2p+1}{2n} + \frac{p(p+1)}{4n^2} \right]. \quad (4.11)$$

It is not hard to verify that the formulas (2.9), (2.10) reproduce this result [all remaining terms in (2.9) vanish].

5. THE TWO-COULOMB-CENTERS PROBLEM

One encounters the problem of two Coulomb centers in various areas of physics.^{28,29} We describe a new approach to this problem, based on the $1/n$ expansion.

The Schrödinger equation has the form

$$\left\{ -\frac{1}{2} \left(\frac{\partial^2}{\partial \rho^2} + \frac{\partial^2}{\partial z^2} \right) + \frac{m^2 - 1/4}{2\rho^2} + V(\rho, z) - E \right\} \Psi = 0, \quad (5.1)$$

where

$$\tilde{V} = -Z_1/r_1 - Z_2/r_2, \quad r_{1,2} = (\rho^2 + s_{1,2}^2)^{1/2},$$

$$s_{1,2} = R/2 \pm z, \quad \rho^2 = (x^2 + y^2)^{1/2},$$

R being the distance between the two centers, $Z_{1,2}$ being their charges and

$$\psi(\mathbf{r}) = \Psi(\rho, z) \rho^{-1/2} \exp(im\phi)$$

being the wave function.

We confine ourselves to states of lowest energy for given m (i.e., $n = m + 1$). After the scale transformation

$$\mathbf{r} = n^2 \mathbf{r}', \quad R = n^2 R', \quad E = \varepsilon n^{-2}, \quad \Psi(\rho', z') = \Phi(n^2 \rho', n^2 z') \quad (5.2)$$

Eq. (5.1) reduces to an equation in which $1/n$ plays the role of the Planck constant \hbar :

$$\left\{ -\frac{1}{2n^2} \left(\frac{\partial^2}{\partial \rho'^2} + \frac{\partial^2}{\partial z'^2} \right) + V(\rho', z') + \left(\frac{1}{2} - \frac{1}{n} + \frac{3}{8n^2} \right) \frac{1}{\rho'^2} - \varepsilon \right\} \Phi = 0 \quad (5.3)$$

(in what follows we omit the prime on the reduced variables ρ', z', R').

In the $n \rightarrow \infty$ limit the particle is localized at the minimum (ρ_0, z_0) of the effective potential $U = V(\rho, z) + 1/2\rho^2$. From the conditions $\partial U / \partial \rho = \partial U / \partial z = 0$ follow the equations

$$Z_1 R = s_2 r_1^3 \rho^{-4}, \quad Z_2 R = s_1 r_2^3 \rho^{-4}, \quad (5.4)$$

which determine the dependence of ρ_0 and z_0 on the parameters $Z_1 R$ and $Z_2 R$ of the problem. The potential $U(\rho, z)$ reduces near the point (ρ_0, z_0) to a two-dimensional anisotropic oscillator, which determines two terms of the $1/n$ expansion

$$\varepsilon^{(0)} = U(\rho_0, z_0) = -(1+2c)/2\rho_0^2, \quad (5.5)$$

$$\varepsilon^{(1)} = 1/2(\omega_1 + \omega_2) - \rho_0^{-2}.$$

Here ω_i are the frequencies of normal vibrations about the equilibrium point

$$\omega_{1,2} = \rho_0^{-2} (1 \pm 3c)^{1/2}, \quad c = \cos \alpha_1 \cos \alpha_2 = s_1 s_2 / r_1 r_2 \quad (5.6)$$

(α_1 and α_2 are the angles of the triangle (Z_1, Z_2, e) at the vertices Z_1 and Z_2). The coefficient $\varepsilon^{(2)}$ is given in Ref. 17. The subsequent corrections $\varepsilon^{(k)}$ can be found by viewing (5.3) as the equation for an anharmonic oscillator.⁴ The algorithm for their calculation reduces to recursion relations, which are easily realized on a computer and permit the reliable calculations of scores of coefficients of the $1/n$ expansion.

The stationary point (ρ_0, z_0) is a local minimum if $\omega_{1,2}^2 > 0$. Physically the answer is obvious in two limiting cases. If $R \rightarrow \infty$ there exist two minima of $U(\rho, z)$: an absolute minimum for $s_1 = R, s_2 = 0, \rho_0 = Z_2^{-1}$ and a local minimum for $s_1 = 0, s_2 = R, \rho_0 = Z_1^{-1}$ (we assume for definiteness that $Z_1 < Z_2$). Corresponding to them we have circular electron orbits, perpendicular to the z axis (connecting the Z_1 and Z_2 charges). On the other hand, if $R \rightarrow 0$ then there is a single minimum at $s_1 = s_2 = 0$ and $\rho_0 = (Z_1 + Z_2)^{-1}$. The disappearance of the local minimum occurs at $R = R_*$, when one of the frequencies ω_i vanishes. Adding to (5.4) the condition $c = 1/3$ we obtain

$$R_* = 3^{1/4} (Z_1 Z_2)^{1/2} \xi, \quad (5.7)$$

where $(Z_1 < Z_2)$

$$\xi = 1 - 3(1 - \xi^2)^{1/2} [(1 + \xi)^{1/2} - (1 - \xi)^{1/2}] / 4\xi, \quad \xi = (Z_1/Z_2)^{1/2}. \quad (5.7')$$

In the case $Z_1 = Z_2 = Z$ the minima are symmetric with respect to the plane $z = 0$. For $R = R_* = 1.299 Z^{-1}$ the two minima merge into one, and for $R < R_*$ the circular orbit lying in the plane $z = 0$ becomes stable. On the other hand if $Z_1 \neq Z_2$, then for $R = R_*$ the local minimum merges with one of the saddle points and disappears. It can be shown that $R_*(Z_1 - Z_2) = R_*(Z_1, Z_2)$. We list numerical values: $R_* = 1.299$ for $Z_1 = Z_2 = 1$; 2.699 for $Z_1 = 1, Z_2 = 2$; 3.489 for $Z_1 = 1, Z_2 = 3, \dots$

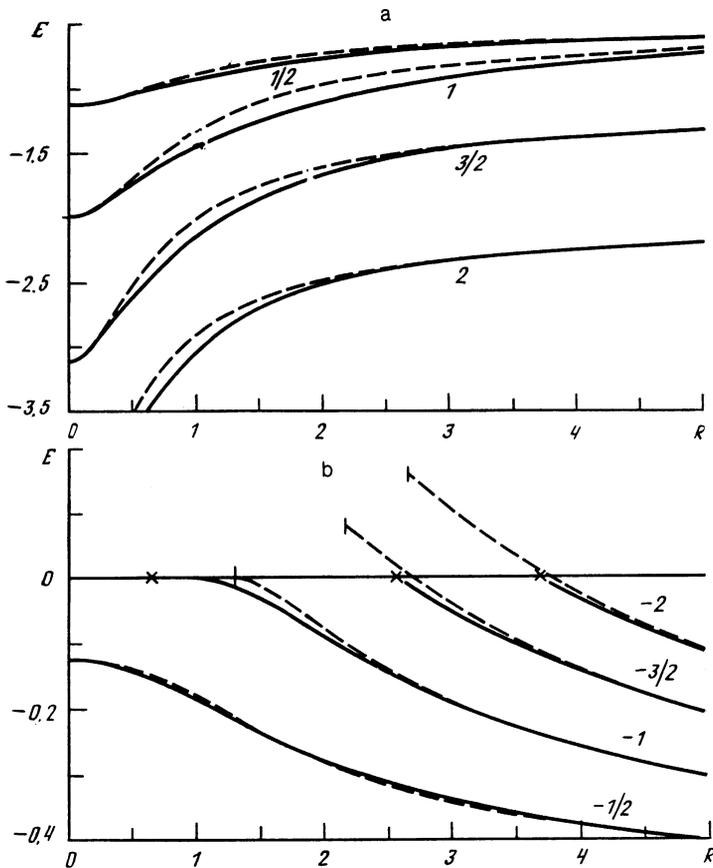


FIG. 2. The energy of the ground term (solid lines) and the classical approximation E_{cl} (dashed lines): a) for $Z_1 = 1$, $Z_2 > 0$; b) for $Z_1 = 1$, $Z_2 < 0$. The curves are labeled by values of Z_2 .

Let us compare the formulas obtained here with other known²⁹ expansions for the two-centers problem. For $R \rightarrow \infty$ there is present in the system a bound state localized near Z_1 . The coefficients $\varepsilon^{(k)}$ may be expanded in inverse powers of R , and $\varepsilon^{(k)} \rightarrow 0$ faster than R^{-k} (at least for $k \leq 7$). Calculations show that the sum of three terms of the $1/n$ expansion gives an approximate value for the reduced energy ε accurate to order R^{-4} . Thus the $1/n$ expansion ensures excellent results for $R \gg 1$.

In the other limiting case ($R \rightarrow 0$) the $1/n$ expansion reproduces the energy $E(R)$ only accurate to order R^2 , however it does not contain terms $\propto R^k \ln R$, present in the expansion of the exact energy.²⁹

We now pass to numerical calculations and compare the exact terms $E(R)$ with the results of the classical approximation $E_{cl}(R) = \varepsilon^{(0)}(n^{-2}R)/n^2$. Here we shall consider the least favorable case $n = 1$.

The solid lines in Fig. 2 describe the energy of the ground state for $Z_2 > 0$ and $Z_2 < 0$, while the dashed lines describe the dependence $E_{cl}(R)$. It is seen that the classical approximation is quite precise (particularly for

$-0.5 \leq Z_2 \leq 0.5$), although the "small parameter" $1/n$ equals unity. In Fig. 2b the crosses denote the values $R = R_{cr}$, for which the level is expelled into the continuum, while the vertical dashes on the curves $E_{cl}(R)$ indicate the values of R_* for which merging of the two classical solutions takes place (analog of $\nu = \nu_*$). In the region $R_* < R < R_{cr}$ (for $Z_2 < -1$) there appear in the system quasistationary states since the local minimum $U(r)$ lies above zero, and the particle may tunnel through the barrier.

In Table II values of the energy of the ground term 1σ obtained by summing the $1/n$ expansion are compared with results of numerical solutions of the Schrödinger equation.⁴⁾ It is seen that the $1/n$ expansion ensures an accuracy needed for most physical applications. By applying more complicated methods of summation it turned out to be possible to determine, starting from Eq. (2.3), also the complex energies of the quasistationary states. The details of the calculation can be found in Ref. 17, which contains a more detailed analysis of the $1/N$ expansion in the problem of two centers as well as results of numerical calculations.

We have considered above only states with $n = m + 1$,

TABLE II. Energy of the ground term in the two-centers problem.

R	$Z_1=Z_2=1$	R	$Z_1=Z_2=1$	R	$Z_1=1, Z_2=-1$	R	$Z_1=1, Z_2=-1$
0.1	1.979	0.5	1.7350	2.0	0.086	4.0	0.2569
	1.9782		1.7350		0.088		0.2583
0.2	1.9285	1.0	1.451	3.0	0.19012	5.0	0.30355
	1.9286		1.4518		0.1901		0.3035

which for $n \rightarrow \infty$ go over into the ground state of the two-dimensional oscillator. However the method can be generalized to excited states as well. Thus, the first correction equals

$$\varepsilon^{(1)} = (n_1 + 1/2)\omega_1 + (n_2 + 1/2)\omega_2 - (n_1 + n_2 + 1)/\rho_0^2, \quad (5.8)$$

where $n_i = 0, 1, \dots$ are the oscillator quantum numbers, and ω_i and ρ_0 have the same meaning as before.

6. THE THREE-BODY PROBLEM

The $1/N$ expansion was first applied to the three-body problem in Ref. 3, where the first three terms $\varepsilon^{(k)}$ were determined (which, however, were insufficient for a satisfactory approximation of the energy). In Ref. 10 the number of calculated coefficients was increased to eleven. Here we shall briefly describe the further development of this method.

We consider the system of three particles in a space of dimension $N_0 = 3$ and introduce the N -dimensional potential

$$V_N(r_{ij}) = \left(\frac{N_0}{N}\right)^2 V\left(\left(\frac{N_0}{N}\right)^2 r_{ij}\right) \quad (6.1)$$

($V_{N_0} \equiv V(r_{12}, r_{23}, r_{31})$). We confine ourselves to S -states, for which the wave function depends only on the three variables r_{ij} . The kinetic energy operator in N -dimensional space will be represented in the form

$$-\frac{1}{2} \sum_{i=1}^3 \frac{1}{m_i} \nabla_i^2 \Psi = T_N \Psi(r_{12}, r_{13}, r_{23}), \quad (6.2)$$

where

$$T_N = T - \frac{N-3}{2} \sum_{i=1}^3 \frac{1}{m_{jk}} \frac{1}{r_{jk}} \frac{\partial}{\partial r_{jk}},$$

$$T = -\frac{1}{4} \sum_{i=1}^3 \frac{1}{m_i} \left[\left(\frac{\partial}{\partial r_{ij}} + \frac{\partial}{\partial r_{ik}} \right) (1 + \cos \theta_i) \left(\frac{\partial}{\partial r_{ij}} + \frac{\partial}{\partial r_{ik}} \right) + \left(\frac{\partial}{\partial r_{ij}} - \frac{\partial}{\partial r_{ik}} \right) (1 - \cos \theta_i) \left(\frac{\partial}{\partial r_{ij}} - \frac{\partial}{\partial r_{ik}} \right) \right], \quad (6.3)$$

$$m_{jk} = m_j m_k / (m_j + m_k), \quad \cos \theta_i = (r_{ij}^2 + r_{ik}^2 - r_{jk}^2) / 2r_{ij}r_{ik},$$

and (i, j, k) is a permutation of the basic triplet $(1, 2, 3)$.

The second term in T_N , linear in derivatives, is eliminated with the help of the transformation

$$S^{-(N-3)/2} T_N S^{(N-3)/2} = T + (N-3)^2 U_c, \quad (6.4)$$

$$U_c = \frac{1}{8} \sum_{i=1}^3 \frac{1}{m_i h_i^2},$$

where S is the area of the triangle with sides r_{12} , r_{13} , and r_{23} , while h_i are its heights ($h_i = 2S/r_{jk}$). In (6.4) only the second term, containing the centrifugal potential U_c , depends on N . Setting $\Phi = S^{(N-3)/2} \Psi$ and $r_{ij} = N^2 s_{ij}$ we arrive at the equation

$$\{N^{-2}T + U_{\text{eff}} - (6N^{-1} - 9N^{-2})U_c - \varepsilon\}\varphi = 0, \quad (6.5)$$

where

$$\varphi(s_{12}, s_{13}, s_{23}) = \Phi(N^2 s_{12}, N^2 s_{13}, N^2 s_{23}),$$

$$U_{\text{eff}} = U + U_c, \quad U(s_{12}, s_{13}, s_{23}) = N_0^2 V(N_0^2 s_{12}, N_0^2 s_{13}, N_0^2 s_{23})$$

and $\varepsilon = N^2 E$. For $N \rightarrow \infty$ the wave function φ becomes localized in the neighborhood of the minimum of U_{eff} , whence

$$\varepsilon^{(0)} = \min U_{\text{eff}}, \quad \varepsilon^{(1)} = \sum_{i=1}^3 \left(n_i + \frac{1}{2} \right) \omega_i - 6U_c, \quad (6.6)$$

with the value U_c taken at the minimum point of U_{eff} . Higher order terms in the $1/N$ expansion

$$\varepsilon = N^2 E = \sum_{k=0}^{\infty} \varepsilon^{(k)} N^{-k} \quad (6.7)$$

take into account corrections due to anharmonicity. These were calculated by means of a recursion procedure⁵⁾ similar, generally speaking, to that used in Ref. 10, even though it differed from it substantially in detail.

We consider a few examples. For a system of three particles with masses $m_1 = m_2 = 1$, $m_3 \gg 1$ and equal pair-interaction potentials

$$V = v(r_{12}) + v(r_{13}) + v(r_{23}) \quad (6.8)$$

the $1/N$ expansion coefficients are given in Table III (for the ground state). To sum the series (6.7) use was made of Padé approximants $[L/M]$, whose values are listed in the last three rows of Table III. The signs, which coincide for all three approximants, may be viewed as reliable. It is seen that for potentials with Coulomb singularity the accuracy of the energy calculation is lower by 1-3 orders, as compared to potentials that are finite at the origin. Let us note that for $v(r) = -r^{-1} \exp(-\mu r)$ the minimum of the potential

TABLE III. Coefficients of the $1/N$ expansion for the three-body problem and its summation with the help of Padé approximants $[L/M]$.

$\varepsilon^{(i)}$, [L/M]	$v(r)$					
	$-1/r$	$-r^{-1} + r$	$-r^{-1} \exp(-r/4)$	$\ln r$	$1/2(r^2 + r^4)$	$-2\exp(-r)$
$\varepsilon^{(0)}$	-7.485	24.56	-2.116	-17.91	51.15	-1.414
$\varepsilon^{(1)}$	-13.94	-31.52	-12.47	-15.20	18.12	-13.44
$\varepsilon^{(2)}$	-20.51	-25.92	-20.91	-3.471	-8.291	1.168
$\varepsilon^{(5)}$	-39.31	-41.31	-39.17	0.05643	3.369	-1.579
$\varepsilon^{(9)}$	-289.3	58.91	-435.7	-74.25	-162.5	-159.2
{3/4}	-1.7917	1.023	-1.1451	-2.59468	6.272481	-0.63410
{4/4}	-1.7911	1.023	-1.1442	-2.59458	6.272475	-0.63420
{5/5}	-1.7915	1.018	-1.1440	-2.59465	6.272477	-0.63417

U_{eff} exists only for $\mu < \mu_* \approx 0.468$, and for $v(r) = -A \exp(-r)$ —for $A > A_* \approx 1.351$.

It is known¹⁰ that for potentials with Coulomb singularity at the origin the energy has a pole at $N = 1$; for example, for a single particle in a Coulomb field we have

$$E_0 = -\frac{2}{(N-1)^2} = -\frac{2}{N^2} \left(1 + \frac{2}{N} + \frac{3}{N^2} + \dots \right). \quad (6.9)$$

With this in mind it becomes convenient to expand in $1/(N-1)$, and not $1/N$. In Table IV we give the results of summing such an expansion for the exotic atom $\bar{p}\bar{p}\alpha$ ($m_1 = m_2 = 1, m_3 = 4$).

In the case of the two-body problem S -states in spaces of dimension $N = 5, 7, 9, \dots$ have the same energy as P -, D -, F -, ...-states in three dimensions. For the three-body problem this is generally not so, but the S -state in five-dimensional space has, as before, the same energy as one of the P -states for $N = 3$.³¹ Using this fact we have calculated the energy of the state $(2p)^2\ ^3P$ (it is more stable against decay by annihilation) with the help of the $1/(N-1)$ expansion for $N = 5$. The Padé approximants give here a substantially higher accuracy than in the preceding case since the expansion parameter is smaller by a factor 2.

With the help of the above method we have calculated energy levels of the three-particle anharmonic oscillator ($v(r) = 1/2r^2 + \lambda r^4$) for $0 < \lambda < 1.5$, as well as the ground state of the screened helium atom and the mesic atom $\mu^- \mu^- \alpha$.

7. THE $1/n$ EXPANSION AND COHERENT STATES

The states which correspond in the limit $n \rightarrow \infty$ to closed circular orbits of the electron are in some sense special: for them the classical approximation retains the qualitative peculiarities of the quantum problem, and often also ensures sufficient accuracy for the calculation of the energy even for $n \sim 1$ (besides the examples discussed in Secs. 2–5 we may also mention the hydrogen atom in electric and magnetic fields). The reason is that the indicated states are (for $n \gg 1$) coherent states, which minimize the uncertainty relations for $\Delta p \Delta q$.

We shall demonstrate this on the example on the hydrogen atom in the absence of external fields, where analytic solutions are known. The wave function of the $|0, 0, m\rangle$ state has the form

$$\begin{aligned} \langle \mathbf{r} | 0, 0, m \rangle &= \frac{1}{\pi^{3/2} n^n n!} (\xi \eta)^l \exp\left(-\frac{\xi + \eta}{2n}\right) \exp(im\varphi) \\ &= i^{l-1} \chi_{nl}(r) Y_{lm}(\theta, \varphi). \end{aligned} \quad (7.1)$$

TABLE IV. Energy of the exotic $\bar{p}\bar{p}\alpha$ atom (in units $e = \hbar = m_p = 1$), obtained by summation of the expansion in powers of $1/(N-1)$.

$[L/M]$	Ground state	$(2p)^2\ ^3P$
$[0/0]$	-2.469	-0.5422
$[3/4]$	-2.322	-0.5653
$[4/4]$	-2.311	-0.5650
$[4/5]$	-2.317	-0.5651

where $l = |m| = n - 1$ and

$$\chi_{nl}(r) = 2^n n^{-(n+1)} [(2n-1)!]^{-1/2} r^n \exp(-r/n).$$

For the operators r and $\hat{p}_r = 1/2[\hat{\mathbf{p}} \cdot (\mathbf{r}/r) + (\mathbf{r}/r) \cdot \hat{\mathbf{p}}] = -(i/r)(\partial/\partial r)r$ we calculate the mean:

$$\begin{aligned} \bar{r} &= n(n+1/2), \quad \Delta r = 1/2 n(2n+1)^{1/2}, \quad \overline{p_r^2} = n^{-2}(2n-1)^{-1}, \\ \Delta p_r \Delta r &= \frac{1}{2} \left(\frac{2n+1}{2n-1} \right)^{1/2}, \quad \Delta p_z \Delta z = \frac{1}{2} \left(\frac{n+1}{n+1/2} \right)^{1/2}, \end{aligned} \quad (7.2)$$

where $\Delta r = (\overline{r^2} - \bar{r}^2)^{1/2}$ is the dispersion. In this way, for $n \gg 1$ the states under consideration minimize the uncertainty relation for the radial and transverse to the orbit plane components of \mathbf{p} and \mathbf{r} , and therefore they are closest to classical mechanics.⁶⁾

For all other states $|nlm\rangle$ the product $\Delta p \Delta q$ exceeds $1/2$. Thus, if $n \rightarrow \infty$ and the radial quantum number $p = n - l - 1 = 0, 1, 2, \dots$ is fixed, then

$$\Delta p_r \Delta r = p + \frac{1}{2} + \frac{1-3p(p+1)}{4n} + O\left(\frac{1}{n^2}\right), \quad (7.3)$$

$$\Delta p_z \Delta z = l - |m| + 1/2 + O(1/n).$$

On the other hand if both quantum numbers n and p are large then $\Delta p \Delta q$ grows proportional to n . For example, for ns -states

$$\Delta p_r \Delta r = 1/2 (n^2 + 2)^{1/2} \approx n/2, \quad \Delta p_z \Delta z = [(5n^2 + 1)/18]^{1/2} \approx 0.53n. \quad (7.4)$$

The Schrödinger equation has exact solutions also in the case of the three-dimensional harmonic oscillator $V(r) = \omega^2 r^2/2$. Analogously to the preceding we obtain ($n \gg 1$)

$$\Delta p_r \Delta r = \begin{cases} p + \frac{1}{2} + \frac{1-3p(p+1)}{32n} + \dots, & p \ll n \\ 2(1-8/\pi^2)^{1/2} n + \dots, & l=0. \end{cases} \quad (7.5)$$

In general (with the exception of states for which p and $l - |m|$ are of order unity) the product of uncertainties $\Delta p_i \Delta q_i \propto n$ for $n \rightarrow \infty$. Therefore the quantum fluctuations increase without bound and the concept of a classical orbit loses meaning.

The minimality property is preserved upon turning on external fields as well as upon changing the internuclear distance in the problem of two centers. We shall illustrate this with the Stark effect as on the example.

In that case the circular orbit corresponding to the states $|0, 0, m\rangle$ with $|m| = n - 1 \gg 1$ is shifted and changes its radius upon turning on the electric field \mathcal{E} . Here

$$\varepsilon^{(0)} = -(1+3\tau^2)(1-\tau^2)^2, \quad r_0 = n^2/(1-\tau^2)^2, \quad (7.6)$$

and the parameter τ is determined from the equation

$$\tau(1-\tau^2)^4 = F. \quad (7.7)$$

Here $F = n^4 \mathcal{E}$, $\varepsilon = 2n^2 E$, and we use atomic units. Whence for $F \rightarrow 0$

$$\tau = F + 4F^3 + \dots, \quad r_0 = n^2(1 + 2F^2 + 19F^4 + \dots),$$

and for $F \rightarrow F_* = 2^{12} \cdot 3^{-9} = 0.2081$ (classical ionization threshold^{13,14}) we have

$$\tau = \frac{1}{3} - \frac{2^{1/2}}{9} \left(\frac{F_* - F}{F_*} \right)^{1/2} + \dots,$$

$$r_0 = \left(\frac{9}{8} n \right)^2 \left[1 - \frac{2^{1/2}}{3} \left(\frac{F_* - F}{F_*} \right)^{1/2} + \dots \right].$$

We confine ourselves to nodeless states (for $1 \ll p \ll n$ the discussion is analogous). Since the Schrödinger equation separates in parabolic coordinates ξ, η, φ we have

$$\langle \mathbf{r} | 0, 0, m \rangle_{n \gg 1} \approx (1/\pi r_0^{1/2}) (\omega_\xi \omega_\eta)^{1/4} \exp \left\{ -1/2 [\omega_\xi \xi^2 + \omega_\eta \eta^2] + im\varphi \right\}. \quad (7.8)$$

Here

$$\begin{aligned} \tilde{\xi} &= \xi - \xi_0, & \tilde{\eta} &= \eta - \eta_0, \\ \xi_0 &= n^2(1-\tau)/(1-\tau^2)^2, & \eta_0 &= n^2(1+\tau)/(1-\tau^2)^2, \end{aligned}$$

and the frequencies of small vibrations about the classical point of equilibrium (ξ_0, η_0) equal

$$\begin{aligned} \omega_\xi &= (1+\tau)(1-\tau^2)^2(1+3\tau)^{1/2}/2n^3, \\ \omega_\eta &= (1-\tau)(1-\tau^2)^2(1-3\tau)^{1/2}/2n^3. \end{aligned} \quad (7.9)$$

Going over in Eq. (7.8) to the coordinates $\tilde{r} = r - r_0$ and $\tilde{z} = z - z_0$ we obtain the two-dimensional Gaussian distribution:

$$\langle \mathbf{r} | 0, 0, m \rangle = \frac{\exp(im\varphi)}{2\pi\sigma r_0^{1/2}(1-\rho^2)^{1/4}} \exp \left[-\frac{\tilde{r}^2 + \tilde{z}^2 + 2\rho\tilde{r}\tilde{z}}{4\sigma^2(1-\rho^2)} \right].$$

From here it follows that \tilde{r} and \tilde{z} have the same dispersions σ and correlation coefficients ρ :

$$\sigma = \left(\frac{\omega_\xi + \omega_\eta}{8\omega_\xi\omega_\eta} \right)^{1/2}, \quad \rho = \frac{\omega_\xi - \omega_\eta}{\omega_\xi + \omega_\eta}. \quad (7.10)$$

Integrating $|\psi|^2$ over one of the variables r or z we obtain a Gaussian packet with dispersion σ independent of the size of ρ . In any event this is the case as long as the solution remains real (i.e., up to $F = F_*$, when the classical solutions collide and then move off into the complex plane^{13,14}).

In this fashion inclusion of the external field does not change the minimality properties ($\Delta p \Delta q \rightarrow 1/2$ for $n \rightarrow \infty$) for the states described in the classical limit by closed orbits. Once this is recognized the applicability of the classical approximation and its high accuracy (see above Secs. 4 and 5) become quite natural.

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APPENDIX 1

Let us discuss refinement of the asymptote (3.2). For $n \rightarrow \infty$

$$c_{nl} = \tilde{c}_{nl} \exp \left\{ -(\beta_1/n + \beta_2/n^2 + \dots) \right\}. \quad (A1)$$

The coefficients β_k are readily found in the cases where the exact solution is known. For example, for the Coulomb potential $x_0 = n^2$, $\omega = 1$, and the integrals (3.3) are equal to $J_0 = 2 \ln n - 1$, $J_1 = 0$. On the other hand, for the exact wave function

$$c_{nl} = \frac{2^{l+1}}{n^{l+2}(2l+1)!} \left[\frac{(n+l)!}{(n-l-1)!} \right]^{1/2}. \quad (A2)$$

Therefore for $n \rightarrow \infty$ and for fixed $p = n - l - 1$ we get

$$\beta_k = \frac{(-1)^k}{2^{k+1}k(k+1)} [B_{k+1}(-p) - 2B_{k+1}(-2p)], \quad (A3)$$

where $B_n(x)$ are the Bernoulli polynomials. In particular, $\beta_1 = (42p^2 + 18p + 1)/48$, $\beta_2 = (10p^3 + 7p^2 + p)/32$, etc.

Let us denote by \check{c}_{nl} the approximation beyond (3.2):

$$\check{c}_{nl} = \tilde{c}_{nl} \exp(-\beta_1/n), \quad (A4)$$

in which terms of order $1/n$ are taken into account. Then $\check{c}_{nl}/c_{nl} = 0.99984, 1.24, 0.99998$, and 1.08 , respectively, for the states $1s, 2s, 2p$, and $3p$. Passage from \tilde{c}_{nl} to \check{c}_{nl} significantly increases the precision of the approximation (since $\tilde{c}_{nl}/c_{nl} = 1.021, 2.33$, and 1.65 for the states $1s, 2s$, and $2p$). The situation is analogous for the harmonic oscillator and for the Tietz potential. In this way calculation of order $1/n$ corrections to (3.2) may substantially broaden the region of applicability of this approximation to states with a number of nodes $p \sim 1$.

From (A3) we have for $p = 0$

$$\beta_k = \frac{B_{k+1}}{2^{k+1}k(k+1)} \approx 2(-1)^{(k-1)/2}(k-1)!(4\pi)^{k-1}. \quad (A5)$$

From here it is seen that the series in (A1) diverges, and the $1/n$ expansion is asymptotic.

- ¹ The series (1.1), as a rule, diverge, therefore to calculate E_{nl} to high accuracy it is necessary to make use of methods of summation of divergent series—such as Padé approximants (PA), etc. (we omit technical details of the calculations referring the reader to Refs. 16 and 17). It is important in practice that in many cases even two–three terms of the $1/N$ expansion yield values of E_{nl} and wavefunctions of acceptable precision for physics.
- ² Thus, values of $\psi^2(0)$ are needed in calculating the $\bar{p}p$ annihilation widths,¹⁸ the decay widths of charmonium,^{19,20} and the four-quark states.²¹ Another example is the calculation of the reaction speed of nuclear fusion in mesomolecules $dd\mu$ and $d\mu$,²² etc.
- ³ These calculations were performed by A. M. Badalyan and S. G. Pozdnyakov, to whom the authors express their sincere appreciation.
- ⁴ The calculation was performed following the program used in Ref. 30.
- ⁵ Because of the highly unwieldy formulas, its description here would be inappropriate (compare with the recurrence relations given in Ref. 16 for a simpler case). We only note that the computation time rapidly increases ($\propto k^8$) with increasing number of coefficients in (6.7) and for $k = 10$ reaches ~ 1 h on the computer CYBER-172.
- ⁶ Compare with the Glauber coherent states $|\alpha\rangle$ for the harmonic oscillator,^{32,33} for which $\Delta p \Delta q = 1/2$ for arbitrary α .

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