$1/N$ expansion for the three-body problem

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(Submitted 9 January 1989)
Yad. Fiz. 50, 945–950 (October 1989)

An expansion in powers of $1/N$, where N is the dimension of space, is used for the calculation of the energy of a quantum-mechanical three-body system. It is proved that the limit $N\to\infty$ corresponds to the classical motion of a rigid configuration of particles in four-dimensional space. The results of the summation of the series in $1/N$ are discussed in the cases of an anharmonic oscillator, the $\mu\mu\alpha$ muonic atom, and screened helium.

1. INTRODUCTION

We first generalize the initial problem to the case of N-dimensional space with variable N. In the limit $N\to\infty$ the particles form a stable rigid configuration. The quantum oscillations around the equilibrium configuration are descried by perturbation theory in powers of $1/N$. The physical dimension $N=3$ is substituted into the final formulas derived in the limit of large N. This often provides a good approximation to the initial theory.

The $1/N$ expansion for the three-body problem was originally developed in Ref. 1 in connection with generalized helium Hamiltonians. In Ref. 1 the first three terms of the $1/N$ expansion were found by means of a method based on the Holstein–Primakoff representation for the pseudospin algebra. In Ref. 2 a calculation of seven coefficients of the $1/N$ expansion for helium and helium-like ions is described, which is carried out by a simpler method and allows the determination of the energy with accuracy of 3–4 decimal points. Later, in Ref. 3 a similar method was used to calculate 11 coefficients for helium. Also, Refs. 4–8 are devoted to various aspects of the $1/N$ expansion for the three-body problem. However, in those references only the lowest orders of the expansion and mainly helium-like systems were considered.

In the present work we establish for the first time that the limit $N\to\infty$ corresponds to the classical motion of a rigid triangular configuration of particles in four-dimensional space. In order to calculate the higher-order coefficients of the $1/N$ expansion, we use the same approach as in Refs. 2 and 3. We consider a three-particle anharmonic oscillator, the $\mu\mu\alpha$ muonic atom, and a screened helium atom as examples. In the latter two cases the results of the summation of the $1/N$ expansion are in agreement with the results of more accurate variational calculations.

2. DESCRIPTION OF THE METHOD

Let us consider a system of particles with masses m_1, m_2, m_3, interacting through the potential $V(r_{23}, r_{31}, r_{12})$ in a space with dimension $N_0=3$, where r_{ij} is the distance between particles i and j. We introduce the potential

$$U(s_{23},\ s_{31},\ s_{12})=N_0^2V(N_0^2s_{23},\ N_0^2s_{31},\ N_0^2s_{12}). \quad (1a)$$

We assume that the generalized N-dimensional potential is

$$V_N(r_{23},\ r_{31},\ r_{12})=N^{-2}U(N^{-2}r_{23},\ N^{-2}r_{31},\ N^{-2}r_{12}). \quad (1b)$$

Obviously, $V_{N_0}=V$.

We confine ourselves here to the consideration of S states, or of the states whose wave functions depend only on the distances between the particles. The action of the N-dimensional kinetic-energy operator on the wave function of the S state can be written as follows:

$$T_N\psi(r_{23},r_{31},r_{12})=\left[T-\frac{N-3}{2}\sum_{i=1}^{3}\left(\frac{1}{m_j}+\frac{1}{m_k}\right)\frac{1}{r_{jk}}\frac{\partial}{\partial r_{jk}}\right]\psi,$$

$$T=-\frac{1}{4}\sum_{i=1}^{3}\frac{1}{m_i}\left[\left(\frac{\partial}{\partial r_{ij}}+\frac{\partial}{\partial r_{ki}}\right)(1+\cos\theta_i)\left(\frac{\partial}{\partial r_{ij}}+\frac{\partial}{\partial r_{ki}}\right)+\left(\frac{\partial}{\partial r_{ij}}-\frac{\partial}{\partial r_{ki}}\right)(1-\cos\theta_i)\left(\frac{\partial}{\partial r_{ij}}-\frac{\partial}{\partial r_{ki}}\right)\right], \quad (2)$$

where j and k are such that (i,j,k) forms an even permutation of the three numbers (1,2,3) and $\cos\theta_i=(r_{ij}^2+r_{ki}^2-r_{jk}^2)(2r_{ij}r_{ki})^{-1}$. We use the system of units in which $\hbar=1$.

The transformation $\Phi=S_\Delta^{(N-3)/2}\psi$, where S_Δ is the area of the triangle with the sides r_{23}, r_{31}, and r_{12}, removes from Eq. (2) the terms linear in the derivatives. The N-dimensional Schrödinger equation with the potential V_N is reduced to the form

$$(T+V_N+(N-3)^2U_C-E)\Phi=0, \quad (3)$$

where

$$U_C=\frac{1}{8}\sum_{i=1}^{3}\frac{1}{m_ih_i^2},$$

$h_i=2S_\Delta/r_{jk}$ are the altitudes of the triangle, and E is the energy. The term in Eq. (3) containing the potential U_C is similar to the centrifugal term $(N-1)(N-3)/(8mr^2)$ for a single particle in a spherically symmetric field.

Let us perform the gauge transformation $r_{ij}=N^2s_{ij}$ and write Eq. (3) in the form

$$(N^{-2}T+U_{eff}+(-6N^{-1}+9N^{-2})U_C-\varepsilon)Y=0, \quad (4)$$

where $Y(s_{23}, s_{31}, s_{12})=\Phi(r_{23}, r_{31}, r_{12})$, $U_{eff}=U+U_C$ is the effective potential, and $\varepsilon=N^2E$ is the reduced energy. The parameter N^{-1} enters into the coefficients of the second derivatives in Eq. (4) in the same manner as the Planck constant.

Let us assume that the effective potential has a minimum. Then, as can be shown, the energy can be expanded in a series of powers of $1/N$:

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$$\varepsilon = \sum_{k=0}^{\infty} \varepsilon_k N^{-k}. \qquad (5)$$

In the classical limit $N \to \infty$ the wave function Y is localized in the vicinity of the minimum of $U_{\rm eff}$, and the energy becomes equal to ε_0, which is the minimum of $U_{\rm eff}$.

In the harmonic-oscillator approximation the function $U_{\rm eff} - \varepsilon_0$ in the vicinity of the minimum can be approximated by the quadratic form of the quantities characterizing the deviation of the coordinates from the equilibrium point. We find from Eq. (4) that $\varepsilon_1 = \varepsilon_{\rm osc} - 6U_{\rm C}$, where $U_{\rm C}$ is taken at the point of the minimum of $U_{\rm eff}$, and

$$\varepsilon_{\rm osc} = \sum_{i=1}^{3} \left(p_i + \frac{1}{2} \right) \omega_i$$

is the energy of the harmonic oscillator with the frequencies ω_i in the state with the quantum numbers p_i $(i = 1,2,3)$.

The higher-order coefficients in the expansion (ε_2, ε_3, ε_4, etc.) represent anharmonic corrections. There exists a recurrence procedure for their calculation, which in the case of the helium atom is described in Ref. 3. In the present work we use a similar procedure for a general potential. It is not given here, because of the rather complicated formulas.

3. THE LIMIT $N \to \infty$ AND CLASSICAL MECHANICS

Let us consider the classical motion of two interacting particles in a central field, i.e., we confine ourselves here to the case $m_3 = \infty$. Just as the motion of a single particle in a central field takes place in a single plane, the motion of two particles takes place within a single four-dimensional space (or in a space with lower dimension), which is spanned by the position vectors of the particles **r** and **s** and the momentum vectors **p** and **q** at some instant of time.

In the four-dimensional space one can form the components of the angular-momentum tensor

$$L_{ij} = r_i p_j - r_j p_i + s_i q_j - s_j q_i$$

two conserved invariants

$$L^2 = {}^1/_4 L_{ij} L_{ij}, \quad M = {}^1/_4 L_{ij} \bar{L}_{ij},$$

where $\bar{L}_{ij} = \frac{1}{2}\varepsilon_{ijkl} L_{kl}$ and ε_{ijkl} is a tensor, antisymmetric in all indices, such that $\varepsilon_{1234} = 1$. The following non-negative invariants are expressed in terms of L^2 and M:

$$K_{\pm}^2 = {}^1/_8 (L_{ij} \pm \bar{L}_{ij})(L_{ij} \pm \bar{L}_{ij}) = L^2 \pm M \geqslant 0,$$

from which it follows that M lies in the range $-L^2 \leqslant M \leqslant L^2$. The invariant M can be written in the form of a determinant:

$$M = {}^1/_2 \varepsilon_{ijkl} r_i p_j s_k q_l.$$

It is obvious that for $M = 0$ the motion of the particles becomes three-dimensional. In the opposite extreme case, when $M = \pm L^2$ and the motion is four-dimensional "up to the limits," $K_{\mp}^2 = 0$, from which $L_{ij} = \pm \bar{L}_{ij}$ for any i and j.

We now describe the classical motion of the particles when the distances between the particles and the force center, and between the particles themselves (r, s, and t, respectively), are conserved. This four-dimensional motion of the particles corresponds to the static solution of the problem in the variables r, s, and t when $r = r^{(0)}$, $s = s^{(0)}$, $t = |\mathbf{r} - \mathbf{s}| = t^{(0)}$, and $(r^{(0)}, s^{(0)}, t^{(0)})$ is the minimum of the effective

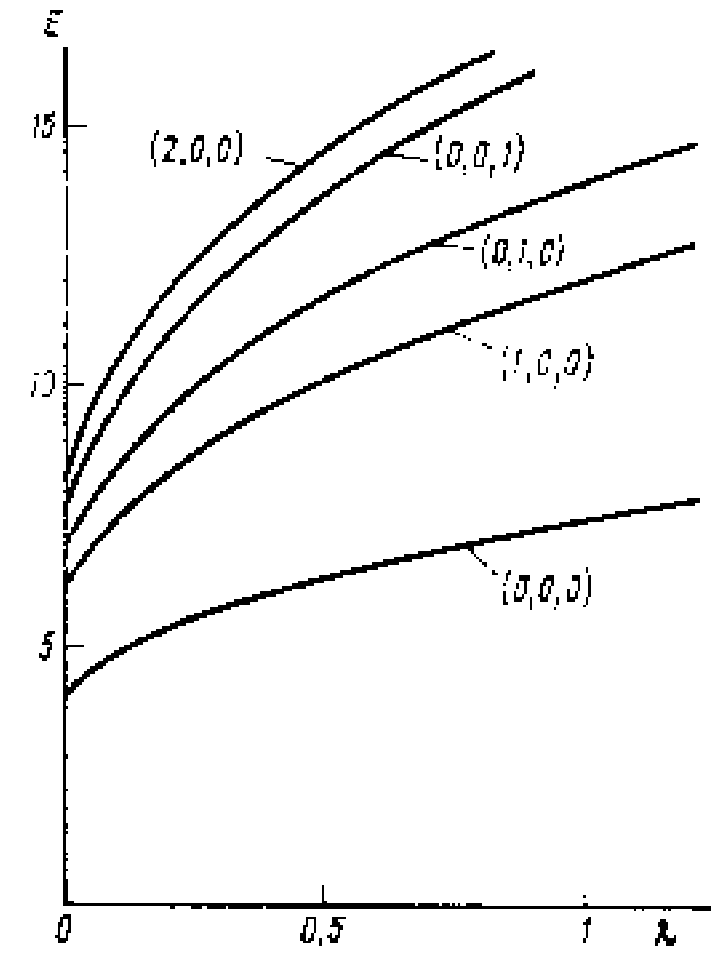

FIG. 1. Energy levels of the three-particle anharmonic oscillator as a function of the anharmonicity parameter.

potential, which arises in the quantum problem in the limit $N \to \infty$ and includes the centrifugal term

$$V_{\rm C}(r, s, t) = (N^2/8)(1/m_1 h_1^2 + 1/m_2 h_2^2),$$

where $h_1 = 2S_\Delta/s$, $h_2 = 2S_\Delta/r$, and $S_\Delta = r_1 s_2 - r_2 s_1$.

Let us specify $L = N/2$ and $M = L^2$ and introduce the axes 1 and 2 of the moving coordinate system in the plane of the triangle, and the axes 3 and 4 in the orthogonal complement to this system. On rotation of the axes 3 and 4 the components L_{13} and L_{14} transform as the components of a two-dimensional vector, so that we can always make $L_{14} = 0$. Taking into account the fact that $L_{ij} = \bar{L}_{ij}$, we find that the only nonzero components of the angular-momentum tensor are

$$L_{13} = L_{42} = -L_{31} = -L_{24} = N/2$$

and that the following equations are valid:

$$r_1 p_3 + s_1 q_3 = L_{13} = L, \quad r_2 p_3 + s_2 q_3 = L_{23} = 0, \qquad (6a)$$

$$r_1 p_4 + s_1 q_4 = L_{14} = 0, \quad r_2 p_4 + s_2 q_4 = L_{24} = -L. \qquad (6b)$$

Substituting the solution of (6) for the unknowns p_3, q_3, p_4, and q_4 into the expression for the kinetic energy, we find

$$T = (p_1^2 + p_2^2)/2m_1 + (q_1^2 + q_2^2)/2m_2 + V_{\rm C}(r, s, t).$$

We fix the momenta and coordinates of the particles at the initial instant of time as follows:

$$p_1 = p_2 = q_1 = q_2 = 0, \quad r = r^{(0)}, \quad s = s^{(0)}, \quad t = t^{(0)}. \qquad (7)$$

Then the total energy coincides with the minimum of the effective potential $V + V_{\rm C}$, and since this energy is conserved, the conditions (7) are satisfied at any instant of time. In this case the distances r, s, and t are conserved.

4. EXAMPLES OF THE 1/N EXPANSION

4.1. Anharmonic oscillator

We consider here the anharmonic oscillator with the particle masses $m_1 = m_2 = 1$, $m_3 = \infty$ and with equal pair interaction potentials $v(r_{ij}) = r_{ij}^2/2 + \lambda r_{ij}^4$, whose sum is the potential V. In Fig. 1 we show the energy levels $E = N^{-2}\varepsilon$ as a function of the anharmonicity parameter λ, obtained by summing the 1/N expansion by the method of Padé approximants. The quantum numbers (p_1, p_2, p_3) are given in brackets near each of the curves.

For $\lambda = 0$ the problem reduces to that of a harmonic oscillator. In this case, of all the coefficients of the $1/N$ expansion only ε_0 for the ground state, and ε_0 and ε_1 for the excited states, are nonzero. The energy of the state (p_1, p_2, p_3) can be calculated exactly:

$$E=(27/N^3)[p_1+N/6 + (p_2+N/6)(\sqrt{3}+1)/2+(p_3+N/6)\sqrt{3}].$$

We note that the factor $27/N^3$ arises because of the coefficient $(3/N)^6$ in front of $r_{ij}^2/2$ in the N-dimensional potential V_N [see Eqs. (1)]. The energies of the states with equal sums $p_1 + p_2 + p_3$ with $p_1 = p_3$ coincide with each other and form a degenerate level.

At large λ the terms λr_{ij}^4 are dominant in the potential. In the case when $v = r_{ij}^4$, the calculations reveal an unexpected relation between the frequencies:

$$\omega_1 : \omega_2 : \omega_3 = 1 : 1.419 : 2.003 \approx 1 : \sqrt{2} : 2.$$

Consequently, for large N the energies of the states with the equal sum $2p_3 + p_1$ are very close, and for them the $1/N$ expansion, because of the strong divergence, is no longer good. We write the energies of some of the low-lying states for the case $v = r_{ij}^4$:

$$E(0, 0, 0)=6.417, \quad E(1, 0, 0)=10.73, \quad E(0, 1, 0)=12.51,$$
$$E(0, 0, 1)=15, \quad E(2, 0, 0)\approx E(0, 0, 1).$$

Only those decimal points are given which are the same for the approximants [3/3], [3/4], and [4/4] and which are reliable.

4.2 Muonic atom $\mu\mu\alpha$

We consider the ground state of the muonic atom $\mu\mu\alpha$ ($m_1 = m_2 = 206.769$, $m_3 = 7293.4$).

In order to take into account the double pole in the energy at $N = 1$ (Ref. 4), we use the expansion in $1/(N-1)$:

$$E'=(N-1)^{-2}\sum_{k=0}^{\infty} \varepsilon_k'(N-1)^{-k},$$

where E' is the energy for the N-dimensional problem with the potential V'_N determined by the expressions (1) with the substitution $N_0 \to N_0 - 1$ and $N \to N - 1$. The corresponding approximants are as follows:

[0/0]′	[3/4]′	[4/4]′	[4/5]′	Variational calculation (Ref. 9)
−549.2	−584.5	−583.05	−583.1	−583.044

As is evident, they are in good agreement with the variational calculation of Ref. 9. In the Coulomb case $V_N = V'_N = V$ and $E = E'$, and therefore the coefficients ε_k and ε'_k are interrelated.

Two terms of the $1/N$ expansion for the $\mu\mu\alpha$ muonic atom were obtained recently in Ref. 8; however, the coefficient $\varepsilon'_1 = -651.1$ differs from the result of the present work ($\varepsilon'_1 = -481.4$) and is, apparently, wrong.

4.3. Screened helium atom

Let us consider a system of three particles with masses $m_1 = m_2 = 1$, $m_3 = \infty$, interacting with each other via the Yukawa potential

$$V(r_1, r_2, r_{12}) = -\frac{2}{r_1}\exp(-\delta r_1) - \frac{2}{r_2}\exp(-\delta r_2) + \frac{1}{r_{12}}\exp(-\delta r_{12}). \tag{8}$$

Just as in the case of a single particle in a Yukawa potential,[10] here we can use perturbation theory in powers of the screening parameter δ:

$$E=\sum_{k=0}^{\infty} E^{(k)}\delta^k.$$

The unperturbed energy $E^{(0)} = -2.903\,724$ is the energy of the ground state of the helium. Since $\partial V/\partial\delta = 3$ at $\delta = 0$, we have $E^{(1)} = 3$. The next two coefficients are expressed in terms of the mean values calculated in Ref. 11:

$$E^{(2)}={}^1/_2(\langle r_{12}\rangle-4\langle r_1\rangle)=-1.147909,$$
$$E^{(3)}=-{}^1/_6(\langle r_{12}{}^2\rangle-4\langle r_1{}^2\rangle)=0.3762487.$$

The results of the calculation of $[2/1](\delta)$ are given in the second column of Table I.

In Table I we present also the results of summation of the expansion in $1/(N-1)$. For $\delta \gtrsim 0.3$ they are in better agreement with the variational calculation[12] (the fourth column of Table I) than with the results of the expansion in δ. We note that the effective potential of the screened helium has a minimum corresponding to the isosceles configuration of the particles, for $\delta < \delta_* \approx 1.2554$.

It is known[13] that the energy of the ground state for $N = 5$ coincides with the energy of the excited state $(2p)^2\,{}^3P$ in a real three-dimensional space. The corresponding results for the screened helium are

δ	0	0.05	0.1	0.15	0.2	0.25
[4/4]′	−0.710505	−0.56969	−0.44596	−0.33784	−0.24434	−0.16450

At $\delta = 0$ the approximate result coincides with the exact result ($-0.710\,500$ from Ref. 14) up to five decimal points.

5. CONCLUSION

We have described a method of obtaining the coefficients of the $1/N$ expansion for a large class of analytic po-

TABLE I. Energy of the ground state of screened helium.

δ	[2/1](δ)	[4/4]′	Variational calculation (Ref. 12)	δ	[2/1](δ)	[4/4]′	Variational calculation (Ref. 12)
0	−2.90372	−2.9039	−2.90372	0.6	−1.449	−1.4563	−1.45856
0.2	−2.34632	−2.3467	−2.34700	0.8	−1.086	−1.106	−1.11033
0.4	−1.8661	−1.8673	−1.86845	1.0	−0.77	−0.804	−0.81821

tentials. The fact that for the two-body problem the limit $N \to \infty$ corresponds to rotation of the bodies around their common center of mass is generalized to the less trivial case of the three-body problem. Tests of the method for some model examples has demonstrated its efficiency, both for the ground state and for some excited states.

The author expresses his gratitude to A. I. Sherstyuk, E. A. Solov'ev, and V. S. Popov for useful discussions.

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Translated by O. Dumbrajs