High Orders of 1/*D*-Expansion for Three-Body Systems

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Introduction

We study the system of three particles in D-dimensional space interacting by means of an analytic potential $V_D(r_{23}, r_{31}, r_{12})$. In the large D limit, the particles form the stable rigid configuration corresponding to a minimum of an effective potential $V_{\text{eff}} = V_D + D^2 U_c$ containing a centrifugal term $U_c = \frac{1}{8}(1/m_1 h_1^2 + 1/m_2 h_2^2 + 1/m_3 h_3^2)$ where h_1, h_2 and h_3 are altitudes in the configurational triangle. The quantum oscillations around the equilibrium are organized as a power series in $1/D$.

The first three coefficients of the $1/D$-expansion for helium Hamiltonians were calculated by Mlodinow and Papanicolaou (1981) using algebraic approach. More direct approach in coordinate representation enables to obtain higher orders of $1/D$-expansion (Sergeev 1983, seven coefficients; Googson and Herschbach 1987, eleven coefficients). The recent effective algorithm (Dunn *et al*. 1994) makes possible to calculate up to 31 coefficients for the ground state of helium. For various non-helium Hamiltonians, high orders of $1/D$-expansion were obtained by Sergeev (1989) and Mur *et al*. (1990).

Although Padé summation of $1/D$-series gives convergent results, the accuracy is not very high because the parameter of the expansion $1/D$ for $D=3$ is not small. So, various ingenious summation methods taking into account both the pole singularity at $D=1$ and the essential singularity at $D=\infty$ were developed (Goodson *et al*. 1992).

In the first part of this communication, we outline the way to establish the singularities of the Borel function to $1/D$-series that lead to factorial divergence of the series

$$E_k \sim \mathrm{Re}(C a^k) k^{-3/2} k!$$

where the parameter *a* is reciprocal to Borel singularity.

In the second part, we develop Darboux - Borel summation procedure that properly accounts for square-root singularity of the Borel function.

In the third part, we discuss the square root singularities of the energy function for *excited* states that lead to non-factorial growth of the expansion coefficients

$$E_k \sim c D_c^k k^{-3/2}$$

where D_c is a branch point joining the levels. To eliminate the divergence for near-crossing levels, we use a simple trick.

1. Singularities of the Borel function as an action along classical trajectories

Typically, the coefficients in $1/D$-expansion grow as factorials, $E_k \sim C a^k k^\beta k!$ (for quasistationary states) or $E_k \sim (C a^k + C^* a^{*k}) k^\beta k!$ (for bound states). To find the parameters C, a and β, the dispersion relations were used between E_k and the integral from the imaginary part of the energy. Particularly, a^{-1} coincides with the action integral standing in the exponent in the quasiclassical formula for decay rate:

$$a^{-1} = \int_{r_0}^{r_1} [2(U_{\text{eff}}(r) - U_0)]^{1/2} dr$$

where $U_{\text{eff}}(r) = D^2 V_{\text{eff}}(D^2 r)$ is a rescaled effective potential, $U_0 = U_{\text{eff}}(r_0)$ is its minimum, and r_1 is a turning point, $U_{\text{eff}}(r_1) = U_0$ (Popov and Sergeev 1993). The above formula is written for one-dimensional effective potential $U_{\text{eff}} = U_{\text{eff}}(r)$ and for quasistationary states only, when the equation $U_{\text{eff}}(r) = U_0$ has a real solution except r_0. In the case of multiple solutions of $U_{\text{eff}}(r) = U_0$, one should take the turning point that yields a dominant term in a decay rate for which the action integral attains a minimum.

For bound states, there is a pair of complex-conjugate turning points, so the large-order asymptotical formula contains two terms.

The extension of the above quasiclassical formula to multidimensional potentials was carried out by Schmid (1986). The application for two-

dimensional effective potentials for axially-symmetric problem of a hydrogen atom in parallel electric and magnetic fields was considered by Popov and Sergeev (1994).

In the case of three-body systems, we deal with a **three-dimensional** quantum decay problem, the number of variables being equal to the number of interparticle distances. The central problem is the solution of the eikonal equation and minimization of the classical action in order to determine the parameter a (and the corresponding singularity of the Borel function $\delta = a^{-1}$).

Two different approaches were used by Popov and Sergeev (1994) (for similar *two*-dimensional problem). The first one is based on the method of characteristics. The classical trajectories in an inverted effective potential are calculated, and a trajectory is chosen which terminates at a stopping point and which represents the most probable escape path. The parameter a equals to the reciprocal of the action along this trajectory. In the second approach, the action is expanded as a perturbation series around the minimum of the effective potential.

For more difficult problem with *three*-dimensional potential, we expect that both of these approaches may be in principle useful. As a test

problem, let us investigate in detail the case of **two-electron atoms**.

The rescaled effective Hamiltonian for such a problem is

$$H(r_1,r_2,\theta,p_1,p_2,p_\theta)=\frac{1}{2}(p_1^2+p_2^2)+\frac{1}{2}(r_1^{-2}+r_2^{-2})(p_\theta^2+\sin^{-2}\theta)$$
$$-\frac{1}{r_1}-\frac{1}{r_2}+\frac{1}{Z}(r_1^2+r_2^2-2r_1r_2\cos\theta)^{-1/2}$$

We are beginning to use the method of characteristics. Our goal is solving six equations of classical motion

$$\frac{dp_k}{dt}=-\frac{\partial H}{\partial x_k},\quad \frac{dx_k}{dt}=\frac{\partial H}{\partial p_k}\qquad (k=1,2,3)$$

where $x_1\equiv r_1$, $x_2\equiv r_2$, $x_3\equiv\theta$, and $p_3\equiv p_\theta$. We integrate the equations of motion from an initial point $(x_1^{(i)},x_2^{(i)},x_3^{(i)})$, $p_1^{(i)}=p_2^{(i)}=p_3^{(i)}=0$ $(U_{\text{eff}}(\mathbf{x}^{(i)})=U_0)$ that is guessed to be a turning point. We choose the final point on the complex classical trajectory so that the distance from $(x_1^{(f)},x_2^{(f)},x_3^{(f)})$ to the point of minimum $(x_1^{(0)},x_2^{(0)},x_3^{(0)})$ be as small as possible. After that, we vary the initial point to force this distance to diminish. Finally, we calculate the extremum of the action $S_0=\int_{t_i}^{t_f}\sum_k p_k\dot{x}_k\,dt$.

This method needs the knowledge of the guess turning point. To calculate it, we use large-Z approximation, when the action is exactly

$$S(r_1, r_2, \theta) = r_1 - 1 - \ln r_1 + r_2 - 1 - \ln r_2 - \ln \sin\theta .$$

At the point of extremum, $\partial S / \partial x_k = 0$. The solution is: $r_1^{(1)} = 1$, $r_2^{(1)} = 1$, $\theta^{(1)} = -\pi/2$ (apart from the point of minimum $r_1^{(0)} = 1$, $r_2^{(0)} = 1$, $\theta^{(0)} = \pi/2$). In fact, the motion from the point $\mathbf{x}^{(1)}$ to the point $\mathbf{x}^{(0)}$ is two-dimensional, because $r_1 = r_2$ at any time. Moreover, $\mathbf{x}$ remains purely real except a vicinity of the singularity at $\theta = 0$ that should be embraced by complex contour. So, the calculations are considerably simplified.

The results are given in the following table.

$S_0 = \delta_p$

Z	Real	Imaginary	Method of calculation
2	0.8849	π	integral of action (exact)
	0.3	3.7	quadratic Padé analysis
3	0.6327	π	integral of action (exact)
	0.3	3.5	quadratic Padé analysis
10	0.2343	π	integral of action (exact)
	-0.05	3.3	quadratic Padé analysis
100	0.0325	π	integral of action (exact)
∞	0	π	integral of action (exact)

The estimates for the singularity of the Borel function obtained by quadratic Padé analysis by Goodson *et al.* (1992) are given in the table also. This singularity is not the singularity nearest to the origin (δ_s) that contribute the dominant term

in the asymptotic formula. The estimates for δ_s were obtained both for the ground state of helium (Goodson *et al.* 1992) and for excited $1s2s\,^3S$ state (Goodson and Watson 1993):

Z	Nearest to the origin singularity: Real	Imaginary	Method of calculation
2	-0.32362	0.10054	QPA, ground state
	-0.308	0.108	QPA, excited state*
	?	?	exact
3	-0.500	0.161	QPA, ground state
	?	?	exact
10	-0.821	0.272	QPA, ground state
	?	?	exact

* For excited states, a^{-1} is the same as for a ground state, but numerical results from QPA may differ because the perturbation series are different.

The exact value of the nearest to the origin singularity remains to be calculated by our approach. We expect to develop the numerical algorithm in near future.

2. Modified Borel summation procedure

The divergence of $1/D$-expansion renders conventional summation method ineffective beyond the lowest orders.

Padé summation considerably improves the convergence by taking into account poles of the function.

Further improvement can be achieved by Padé - Borel summation that properly accounts for factorial growth of the expansion coefficients. The method reduces to construction of Padé approximant to the Borel function and subsequent integration of the approximant with the decaying exponent.

The increase of the coefficients of the $1/D$-expansion like $a^k k^{-3/2} k!$ leads to the square-root singularity in the Borel function at $z_0 = a^{-1}$. We can establish the position of this singularity by evaluation of the classical action along the most probable escape path.

Here, we propose to use the approximants of the form

$$\tilde{f}(z) = \frac{B}{A} + \frac{C}{A}(z_0 - z)^{1/2}$$

where A, B and C are polynomials of degree N obeying the relation

$$Af(z) - B - C(z_0 - z)^{1/2} = O(z^{3N+2}).$$

The same approximants were used by Goodson and Watson (1993) to sum the *energy* function for $|010\rangle$ state of helium. They were called Darboux approximants.

As an illustration, let us examine quasistationary states of a hydrogen atom in parallel electric and magnetic fields. We use $1/n$-expansion that is equivalent to "shifted" expansion in powers of $1/(D+1)$. We calculate quadratic Padé approximants (used instead of ordinary Padé approximants in case of quasistationary states), Padé - Borel approximants, and Darboux - Borel approximants constructed from the same number of terms in the expansion (5 terms or 11 terms). The results are given in the following two tables, for magnetic fields B=0.5 and B=1, correspondingly. The results that are nearest to the numerical solution found by Anokhin and Ivanov (1983) were underlined. These best results are exactly Darboux - Borel approximants in most cases.

Thus, Darboux - Borel approximants take full advantage from the known singularity structure of the Borel function, and so the results appear to be more accurate than the results by another summation procedures (quadratic Padé and Padé - Borel).

3. Branch points, avoided crossings, and degenerate perturbation theory for excited states

For the excited $1s2s\,^1S$ state of helium, $1/D$-series appears to be strongly divergent because of the presence of a square-root branch point at

$\delta_s = -0.011386007$ (Goodson and Watson 1993). Here, we explain the origin of this singularity as a result of crossing with another excited level.

To justify our conjecture, we perform analytic continuation of the vibrational part of the energy, $\varepsilon = (E - E_0)D$ along the contour embracing the branch point. For this purpose, we use quadratic Padé approximants (see a figure). The quadratic Padé approximant has two branches which are the roots of quadratic equation. The main branch behaves as $\varepsilon = -0.631 - 41.6D^{-1} + \ldots$ when $\delta = 1/D \to 0$ (solid line). One can see that quadratic PA gives correct value to the branch point δ_s. Moreover, the second (supplementary) branch of quadratic PA may be continued backward from the branch point to the origin (dashed line), and it gives $\varepsilon' = 1.04 + O(D^{-1})$. It exactly coincides with the vibrational energy for the state of the oscillator with quantum numbers (200): $E_1^{|200\rangle} = 1.04046$. So, one has to assign (200) quantum numbers to the second branch of $|010\rangle$ energy function (corresponding to $1s2s\,^1S$ state).

The origin of this phenomenon is a Fermi-like resonance between molecular-like vibrational excitations. If the charge of the nucleus assumes non-integer value $Z_c = 157$, then the first two frequencies of vibrations are related as 1:2. So, one can expect near-degeneracy of the levels ($n_1 = 0$, $n_2 = 1$) and ($n_1 = 2$, $n_2 = 0$) for the nearest to

Z_c integer charge $Z = 2$ corresponding to helium. Since near-degenerate states are highly sensitive to perturbation caused by anharmonic terms in a potential, the $1/D$-expansion diverges.

A convenient way to overcome the divergence is to consider the sum and the product of the energies. As their expansions have no more branch point singularity, they can be easily summed. Finally, the energies can be calculated from the corresponding quadratic equation.

Recently, we have studied in detail the pattern of energy levels, avoided crossings, and branch points for a hydrogen atom in a magnetic field. Such system has all essential features of a general non-separable problem. The enclosed paper was submitted to *J. Phys. B*.

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