Perturbation theory at large orders for a potential with degenerate minima

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(Received 15 March 1977)

Perturbation theory at large orders for a potential with degenerate minima differs from other cases discussed in previous works. The pseudoparticle which interpolates between the two classical minima does not correspond to a periodic path, and one has to consider here pseudoparticle-antipseudoparticle configurations. As expected, the result is a divergent perturbation series with no sign alternance at large orders.

I. INTRODUCTION

In recent articles[1] it has been shown how to characterize the large-order behavior of perturbation theory in the ϕ^4 field theory through the contribution of pseudoparticles to the path integral. This method has been generalized[2] to a polynomial interaction for arbitrary boson theories. In particular an explicit formula has been given in the case of quantum mechanics for the ground-state energy. In this study an important case had remained unsolved, the case of a classical potential with degenerate minima, in which a divergent result was found. In this article we show how the expression found in the general case has to be modified when the potential has nearly degenerate minima.

The main problem was the following: The pseudoparticle solution to the classical Euclidean equation of motion for the anharmonic oscillator, which governs the large-order behavior, has to give a finite contribution to the action, and to satisfy periodic boundary conditions. In the case of degenerate minima such a solution does not exist. In particular the well-known pseudoparticle which interpolates between the two minima and corresponds to the quantum-mechanical tunneling does not satisfy this last condition. Also if one removes the degeneracy by adding a small term of order ϵ to the potential one finds now a classical solution which has no limit when ϵ goes to zero.

We shall show that if we expand around an interacting pseudoparticle-antipseudoparticle path configuration, we can obtain the correct result after we integrate over a parameter describing the separation of the pseudoparticle-antipseudoparticle pair. By the same method a formula which interpolates when ϵ goes to zero between the degenerate and nondegenerate case is obtained.

The pseudoparticle-antipseudoparticle path configuration does not correspond to a solution of the equation of motion, but the derivative of the action with respect to the path vanishes exponentially when the separation between the pseudoparticles goes to infinity. This more precise analysis confirms the result, indicated in Ref. (2), that the perturbation series in the case of degenerate minima is not Borel-summable, all terms at large orders having the same sign, so that the following problem remains: How does one extract the true ground-state energy from perturbation series?

Numerical calculations have been made in order to check the results. For the simplest double-well potential $V(x)=\frac{1}{2}x^2(1-gx)^2$, the first 73 terms of the expansion of the ground-state energy have been computed and they are listed in Table I. They agree with the asymptotic formula (see Table II)

$$E_K=-K!\,3^K\frac{3}{\pi}\left[1-\frac{103}{36}\frac{1}{K}+O\left(\frac{1}{K^2}\right)\right]$$

in which the coefficient of $1/K$ is merely a numerical estimate while the other terms will be derived below.

II. PSEUDOPARTICLE-ANTIPSEUDOPARTICLE PAIR IN A SIMPLE MODEL

The principles of the large-order calculations of energy levels have been described in previous articles,[1,2] to which the reader is referred for a more detailed exposition. The ground-state energy is taken as the zero-temperature limit

$$E=E_0+\lim_{\beta\to\infty}\left(-\frac{1}{\beta}\ln\frac{\operatorname{Tr}e^{-\beta H}}{\operatorname{Tr}e^{-\beta H_0}}\right). \tag{1}$$

Let us write

$$H=\tfrac{1}{2}p^2+\frac{1}{g^2}V(gx), \tag{2}$$

in which $x=0$ is a minimum of V normalized to

$$V(x)\underset{x\to 0}{\sim}\tfrac{1}{2}x^2, \tag{3}$$

and $H_0=\frac{1}{2}(p^2+x^2)$.

The ratio of traces (1) is expressed by the Feynman-Kac path integral over periodic trajectories of period β ("motions" here refer to imaginary time). The order K of perturbation theory is projected out by a contour integral in the g plane:

$$\left(\frac{\mathrm{Tr}e^{-\beta H}}{\mathrm{Tr}e_{-\beta H_0}}\right)_{(K)}=N\int_{x(\beta/2)=x(-\beta/2)}\mathfrak{D}x(t)\int\frac{dg}{2i\pi g^{K+1}}\exp\left\{-\int_{-\beta/2}^{\beta/2}dt\left[\tfrac{1}{2}\dot{x}^2(t)+\frac{1}{g^2}V(gx(t))\right]\right\}. \tag{4}$$

For large K we have to solve the equations of motion

$$\ddot{x}_c=V'(x_c), \tag{5a}$$

$$g_c^2=\frac{2}{K}\int_{-\beta/2}^{\beta/2}dt\left[\tfrac{1}{2}\dot{x}_c^2+V(x_c)\right]. \tag{5b}$$

Periodic motions correspond to fixed energies $\mathcal{E}$

$$\beta=2\int_{x_-}^{x_+}\frac{dx}{[2V(x)+\mathcal{E}]^{1/2}} \tag{6}$$

in which x_- and x_+ are the zeros of $2V+\mathcal{E}$,

$$\tfrac{1}{2}\dot{x}^2=V(x)+\mathcal{E}, \tag{7a}$$

$$g_c^2=\frac{2}{K}\left[\beta+2\int_{-\beta/2}^{\beta/2}V(x)dt\right]. \tag{7b}$$

If the potential had a lower minimum at some other location $x=1$, in the large-β limit we would select the zero-energy trajectory which leaves the origin at time $-\infty$, reflects over the potential, and returns to the origin at time $+\infty$. However, if the potential has a minimum at $x=1$ degenerate with $x=0$, i.e., $V(1)=0$, $V'(1)=0$, $V''(1)>0$, the particle leaving the origin would reach $x=1$ after an infinite time and would never come back. Therefore we have to use, instead of a solution to the equations of motion (7), something which is very close to a solution in which the particle is allowed to come back to the origin. This leads to the pseudoparticle-antipseudoparticle picture which we shall describe in a simple example.

Consider the double-well potential

$$V(x)=\tfrac{1}{2}x^2(1-x)^2. \tag{8}$$

The pseudoparticle solution

$$x_I=(1+e^{-(t-t_0)})^{-1} \tag{9}$$

leaves $x=0$ at $t=-\infty$ and reaches $x=1$ at $t=+\infty$. The Euclidean action corresponding to this particular path is equal to (a factor $1/g^2$ given by the rescaling $x\to x/g$ is left over)

$$A(x_I)=1/6, \tag{10}$$

in which the action of a path is defined as

$$A(x)=\int dt[\tfrac{1}{2}\dot{x}^2+V(x)]. \tag{11}$$

Let us thus consider the motion

TABLE I. The 73 first E_K's.

K	$-E_K$	K	$-E_K$	K	$-E_K$
1	1	26	$8.642\,4175\times10^{38}$	51	$3.003\,1494\times10^{90}$
2	4.5	27	$7.036\,2748\times10^{40}$	52	$4.690\,6127\times10^{92}$
3	4.45×10	28	$5.938\,3598\times10^{42}$	53	$7.466\,7886\times10^{94}$
4	$6.266\,25\times10^{2}$	29	$5.188\,8735\times10^{44}$	54	$1.210\,9783\times10^{97}$
5	$1.103\,1375\times10^{4}$	30	$4.688\,8201\times10^{46}$	55	$2.000\,2728\times10^{99}$
6	$2.288\,8556\times10^{5}$	31	$4.376\,9367\times10^{48}$	56	$3.363\,9531\times10^{101}$
7	$5.419\,8081\times10^{6}$	32	$4.216\,5181\times10^{50}$	57	$5.758\,1229\times10^{103}$
8	$1.435\,9941\times10^{8}$	33	$4.187\,9506\times10^{52}$	58	$1.002\,8810\times10^{106}$
9	$4.201\,5543\times10^{9}$	34	$4.284\,7327\times10^{54}$	59	$1.776\,7532\times10^{108}$
10	$1.344\,8427\times10^{11}$	35	$4.511\,8344\times10^{56}$	60	$3.201\,0318\times10^{110}$
11	$4.675\,5394\times10^{12}$	36	$4.885\,8777\times10^{58}$	61	$5.862\,9761\times10^{112}$
12	$1.755\,4856\times10^{14}$	37	$5.437\,0504\times10^{60}$	62	$1.091\,4290\times10^{115}$
13	$7.083\,9072\times10^{15}$	38	$6.213\,0365\times10^{62}$	63	$2.064\,4751\times10^{117}$
14	$3.059\,3930\times10^{17}$	39	$7.285\,6538\times10^{64}$	64	$3.966\,9052\times10^{119}$
15	$1.408\,8306\times10^{19}$	40	$8.761\,4543\times10^{66}$	65	$7.741\,3461\times10^{121}$
16	$6.893\,9952\times10^{20}$	41	$1.079\,8402\times10^{69}$	66	$1.533\,9152\times10^{124}$
17	$3.573\,7663\times10^{22}$	42	$1.363\,2129\times10^{71}$	67	$3.085\,3696\times10^{126}$
18	$1.956\,9889\times10^{24}$	43	$1.761\,7563\times10^{73}$	68	$6.298\,5082\times10^{128}$
19	$1.129\,0671\times10^{26}$	44	$2.329\,5604\times10^{75}$	69	$1.304\,6661\times10^{131}$
20	$6.846\,5421\times10^{27}$	45	$3.150\,1152\times10^{77}$	70	$2.741\,5829\times10^{133}$
21	$4.353\,8669\times10^{29}$	46	$4.354\,0274\times10^{79}$	71	$5.843\,2635\times10^{135}$
22	$2.897\,5942\times10^{31}$	47	$6.148\,4421\times10^{81}$	72	$1.262\,9199\times10^{138}$
23	$2.014\,3376\times10^{33}$	48	$8.866\,5286\times10^{83}$	73	$2.767\,4449\times10^{140}$
24	$1.460\,1340\times10^{35}$	49	$1.305\,1790\times10^{86}$		
25	$1.101\,8308\times10^{37}$	50	$1.960\,3573\times10^{88}$		

$$x_{I,A}=\begin{cases}(1+e^{-(t-t_0)})^{-1}, & t<\frac{1}{2}(t_0+t_1) \quad (12a)\\ (1+e^{(t-t_1)})^{-1}, & t>\frac{1}{2}(t_0+t_1). \quad (12b)\end{cases}$$

The value of the corresponding action is very close to $2A(x_I)=\frac{1}{3}$ if the pseudoparticle (12a) and antipseudoparticle (12b) are widely separated and $\frac{1}{3}$ is the limit of the action for periodic paths of long period and vanishingly small energy. If we call θ the separation

$$\theta=(t_1-t_0), \tag{13}$$

for large θ

$$A(x_{I,A})=\tfrac{1}{3}-e^{-\theta}. \tag{14}$$

Let us now substract from the potential $V(x)$ a small ϵx^2 term which removes the degeneracy between the two minima. The solution of the equations of motion remains very close to (12) and, since $x_{I,A}$ differs from zero only on a region of size θ, we have now

$$A(x_{I,A})=\tfrac{1}{3}-e^{-\theta}-\epsilon\theta. \tag{15}$$

For ϵ finite we have studied in a previous article[2] the large-order behavior of the ground-state energy

$$E=\sum_0^\infty E_K g^{2K}, \tag{16}$$

$$E_K \underset{K\to\infty}{\sim} -\frac{\pi^{-3/2}}{\sqrt{2\epsilon}}\,\Gamma(K+\tfrac{1}{2})(\tfrac{1}{3}+\epsilon\ln\epsilon)^{-(K+1/2)}. \tag{17}$$

This result increases without bound if ϵ goes to zero. However, we are interested in the limit in which ϵ goes to zero before K goes to infinity, and in fact we shall determine the crossover region in which K is large, ϵ is small, but $K\epsilon$ is finite. We shall not worry in the following about constant normalization factors which will be fixed at the end in order to reproduce the result (17).

The quasisolution (12) depends on two collective variables t_0 and t_1, or rather on the center of mass $\frac{1}{2}(t_0+t_1)$ and on the separation $\theta=t_1-t_0$. The Jacobian of the change of variables to collective coordinates in the path integral will have off-diagonal terms involving the scalar product of $\partial x_{IA}/\partial t_0$ with $\partial x_{IA}/\partial t_1$. For large θ the overlap of these two functions is exponentially small and thus, up to exponentially small terms, the Jacobian is θ independent. Small fluctuations around (12) involve, apart again from exponentially small factors, the square of the determinant corresponding to the integration over the fluctuations around the one-pseudoparticle solution. Since this determinant is a pure constant, we find that the measure of the integration over the two collective variables is essentially constant. This is specific to this simple potential as will be shown below. The integration over the center of mass suppresses as in all problems the β factor of Eq. (1), and once we have integrated over the g^2 fluctuations we are left with a one-variable integral over θ for E_K:

$$E_K \underset{K\to\infty}{\sim} NK!\int\frac{d\theta}{(\frac{1}{3}-e^{-\theta}-\epsilon\theta)^K}, \tag{18}$$

in which the normalization constant N will be determined later.

The g integration implies that a complex contour, which will be specified below, is chosen in the θ plane. It is convenient to use the variable $z=e^{-\theta}$, in which the integral (18) reads

$$E_K \underset{K\to\infty}{\sim} NK!\int\frac{dz}{z}(\tfrac{1}{3}-z+\epsilon\ln z)^{-K}. \tag{18$'$}$$

When K goes to infinity at fixed ϵ there is a saddle point at $z_c=\epsilon$. However, if ϵ goes to zero first the integrand becomes singular at the saddle point and the steepest-descent method is no longer applicable. For ϵK finite the relevant range of integration in the z plane is of order ϵ. Up to negligible corrections one can thus integrate in the variable $\zeta=z/\epsilon$ along a contour C which surrounds the whole cut across the negative real ζ axis:

$$E_K \underset{K\to\infty}{\sim} NK!\int_C\frac{d\zeta}{\zeta}(\tfrac{1}{3}+\epsilon\ln\epsilon-\epsilon\zeta+\epsilon\ln\zeta)^{-K}. \tag{19}$$

The quantity

$$A_c(\epsilon)=\tfrac{1}{3}+\epsilon\ln\epsilon+0(\epsilon) \tag{20}$$

is the action for the periodic zero-energy pseudoparticle, and in the large-K, finite-ϵK limit we obtain

$$E_K \underset{K\to\infty}{\sim} \frac{NK!}{[A_c(\epsilon)]^K}\int_C\frac{d\zeta}{\zeta}e^{[\epsilon K/A_c(\epsilon)](\zeta-\ln\zeta)}. \tag{21}$$

This last integral is elementary and yields

$$E_K \underset{K\to\infty}{\sim} N\frac{K!}{[A_c(\epsilon)]^K}F\left(\frac{\epsilon K}{A_c(\epsilon)}\right), \tag{22}$$

$$F(x)=\pi\frac{e^{-x}x^x}{\Gamma(x+1)}. \tag{23}$$

If we now use (17) to fix the normalization we end up with

$$E_K \underset{K\to\infty,\,\epsilon K\text{ finite}}{\sim} -\frac{1}{\pi^2}\frac{K!}{[\frac{1}{3}-\epsilon\ln(1/\epsilon)]^{K+1}}F\left(\frac{\epsilon K}{A_c(\epsilon)}\right). \tag{24}$$

In particular for the $\epsilon=0$ limit of broken symmetry we obtain

$$E_K \underset{K\to\infty}{\sim} -K!\,3^K\frac{3}{\pi}\left[1+0\left(\frac{1}{K}\right)\right]. \tag{25}$$

We see that, as had been anticipated in Ref. 2, at high orders all the terms of the series have the same sign, and thus the Borel transform of the

TABLE II. $U_K = -E_K/3^K K!$ and $V_K = (K+1)U_{K+1} - KU_K$. The large-$K$ limit of V_K and U_K are identical but the $1/K$ corrections are absent in V_K; they should both approach the limit $3/\pi = 0.954\,930$. At order 73 the expected error is a few percent in U_K and less than 10^{-3} in V_K.

K	U_K	V_K
40	0.883 2445	0.956 544
41	0.885 0323	0.956 453
42	0.886 7328	0.956 367
43	0.888 3522	0.956 293
44	0.889 8963	0.956 222
45	0.891 3702	0.956 152
46	0.892 7785	0.956 097
47	0.894 1257	0.956 036
48	0.895 4155	0.955 984
49	0.896 6516	0.955 932
50	0.897 8372	0.955 896
51	0.898 9756	0.955 848
52	0.900 0693	0.955 804
53	0.901 1209	0.955 774
54	0.902 1330	0.955 736
55	0.903 1076	0.955 703
56	0.904 0468	0.955 677
57	0.904 9526	0.955 639
58	0.905 8265	0.955 623
59	0.906 6705	0.955 589
60	0.907 4858	0.955 566
61	0.908 2740	0.955 549
62	0.909 0365	0.955 518
63	0.909 7723	0.955 502
64	0.910 4888	0.955 482
65	0.911 1810	0.955 467
66	0.911 8520	0.955 442
67	0.912 5026	0.955 431
68	0.913 1339	0.955 410
69	0.913 7466	0.955 404
70	0.914 3417	0.955 380
71	0.914 9197	0.955 369
72	0.915 4815	0.955 361
73	0.916 0278	

energy has a singularity on the integration path. As a final remark let us note that the continuation of (24) for $\epsilon < 0$ does describe the crossover to the stable oscillating regime studied in Ref. 2. Indeed if $\epsilon \to |\epsilon| e^{i\pi} A_c(\epsilon) \to a - i\pi|\epsilon| \simeq a e^{-\pi|\epsilon/a|}$, in which $a = \frac{1}{3} + |\epsilon \ln|\epsilon||$, the phases of A_c^K and of x^x in $F(x)$ [Eqs. (22), (23)] cancel each other; $1/\Gamma(1+x)$ is replaced by $-\Gamma(-x)(\sin\pi x/\pi)$. Thus in the $\epsilon K \to \infty$ limit we do recover the limit studied in (2):

$$E_K = \frac{1}{\pi}\left(\frac{2}{K|\epsilon|\pi}\right)^{1/2} a^{-(K+1/2)} \sin 3\pi K|\epsilon| \,.$$

III. GENERAL POTENTIAL

For a general analytic potential possessing two degenerate minima the calculations are very similar. The only difference lies, as we shall see, in the character of the integration measure over the pseudoparticle-antipseudoparticle separation.

Consider the Hamiltonian

$$H = \tfrac{1}{2}p^2 + \frac{1}{g^2}V(gx) \tag{26}$$

with a potential V possessing two lowest minima

$$\begin{aligned} &x = 0, \quad V'(0) = 0, \quad V''(0) = 1\,, \\ &x = a, \quad V'(a) = 0, \quad V''(a) = v^2\,. \end{aligned} \tag{27}$$

Again, the zero-energy pseudoparticle tunneling from 0 to a does not come back to the origin, and let $A(x_I)/g^2$ be the value of the corresponding action

$$A(x_I) = \int_0^a dx[2V(x)]^{1/2} \tag{28}$$

As before we consider a pseudoparticle going from 0 to a staying at $x = a$ for a large time θ and returning to the origin. The corresponding action is

$$A_c = \frac{1}{g^2}[2A(x_I) - ce^{-v\theta}]\,, \tag{29}$$

in which c is some constant which depends on the details of the potential.

If we add again a small $-\epsilon x^2$ to the potential the action becomes

$$A_c = \frac{1}{g^2}[2A(x_I) - Ce^{-v\theta} - \epsilon\theta a^2]\,, \tag{30}$$

since the particle is near $x = a$ during a time interval of size θ.

The only problem is to determine the measure of the θ integration. Since the curvature around the two minima 0 and a are different, the determinant of the fluctuations,

$$\det\left[-\frac{d^2}{dt^2} + V''(x_{IA})\right],$$

contains in addition to the two wells around t_0 and t_1 a square-well part of width θ.

The integration over the fluctuations around t_0 and t_1 give a θ-independent contribution absorbed into the normalization. In addition there is a third piece given by the scattering off the square well (Fig. 1). The phase shifts are easy to compute

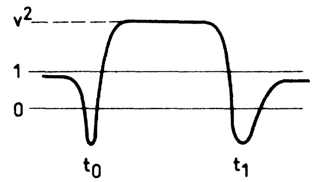

FIG. 1. The potential for the small fluctuations around the classical path.

and they give a Fredholm determinant proportional to $e^{\theta(v-1)}$.

The measure of the θ integration is thus the inverse of the square root of this number, i.e., $e^{(1-v)\theta/2}$. Therefore the K^{th}-order contribution to the ground-state energy (expanded in powers of g^2) is

$$E_K \underset{K\to\infty}{\sim} NK! \int d\theta \frac{e^{(1-v)\theta/2}}{[2A(x_I) - Ce^{-v\theta} - \epsilon\theta a^2]^K} . \tag{31}$$

Translating θ of $-(1/v)\ln\epsilon$, and taking the limit $K\to\infty$, with ϵK finite, we obtain

$$E_K \underset{K\to\infty}{\sim} NK!\, \epsilon^{(v-1)/2v} \int \frac{d\theta\, e^{[(1-v)/2v]\theta}}{[A_c(\epsilon)]^K} e^{-\rho(\theta+e^{-\theta}-1)}, \tag{32}$$

in which

$$A_c(\epsilon) = 2A(x_I) + \frac{a^2}{v}\epsilon\ln\epsilon , \tag{33a}$$

$$\rho \equiv \frac{\epsilon K a^2}{vA_c(\epsilon)} . \tag{33b}$$

The integration over θ may be performed as before and we obtain

$$E_K \underset{K\to\infty}{\sim} NK! \frac{\epsilon^{(v-1)/2v}}{[A_c(\epsilon)]^K} \frac{\rho^{\rho+(1-v)/2v} e^{-\rho}}{\Gamma(\rho+(1+v)/2v)} . \tag{34}$$

The normalization of (34) may be obtained from the knowledge of the $\rho\to\infty$ limit given in (2). The result is

$$N = -\sum_{\substack{\text{leading}\\ \text{saddle}\\ \text{points}}} \frac{2^{1/2v-1/2}a^2}{\pi\sqrt{v}A_c} \exp\left[\int_0^a dx\left(\frac{1}{[2V(x)]^{1/2}} + \frac{1}{x[(x/a)^v - 1]}\right)\right] . \tag{35}$$

For the potential

$$v(x) = \tfrac{1}{2}x^2(1-x^M)^2 \tag{36}$$

there are two degenerate saddle points for M even and only one for M odd.

In the degenerate case $\epsilon = 0$ we thus obtain

$$E_K \underset{K\to\infty}{\sim} -\sum_{\substack{\text{leading}\\ \text{saddle}\\ \text{points}}} \frac{K!}{[2A(x_I)]^{K+1/2v+1/2}} K^{(1-v)/2v} \frac{2^{1/2v-1/2}a^{1+1/v}}{\pi v^{1/2v}\Gamma(\frac{1}{2}+1/2v)} \exp\left[\int_0^a dx\left(\frac{1}{[2V(x)]^{1/2}} + \frac{1}{x[(x/a)^v - 1]}\right)\right] . \tag{37}$$

For the potential (36) this gives

$$E_K \underset{K\to\infty}{\sim} -\frac{1}{2} \frac{3+(-)^M}{\pi M^{1/2M}} \frac{K!K^{(1-M)/2M}}{\Gamma(\frac{1}{2}+1/2M)} \frac{2^{1/2M-1/2}}{[M/(M+2)]^{K+1/2M+1/2}} . \tag{38}$$

ACKNOWLEDGMENT

It is pleasure to thank R. Seznec who actively participated to the numerical computations.

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