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Ulrich D. Jentschura

Missouri University of Science and Technology, ulj@mst.edu

Jean Zinn-Justin

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Instantons in quantum mechanics and resurgent expansions

Ulrich D. Jentschura^{a,b}, Jean Zinn-Justin^{c,d}

^a *Physikalisches Institut der Universität Freiburg, Hermann-Herder-Straße 3, D-79104 Freiburg im Breisgau, Germany*

^b *National Institute of Standards and Technology, Gaithersburg, MD 20899-8401, USA*

^c *DAPNIA/DSM (Département d'astrophysique, de physique des particules, de physique nucléaire et de l'instrumentation associée), Commissariat à l'Énergie Atomique, Centre de Saclay, F-91191 Gif-sur-Yvette, France*

^d *Institut de Mathématiques de Jussieu-Chevaleret, Université de Paris VII, F-75251 Paris Cedex 05, France*

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Abstract

Certain quantum mechanical potentials give rise to a vanishing perturbation series for at least one energy level (which as we here assume is the ground state), but the true ground-state energy is positive. We show here that in a typical case, the eigenvalue may be expressed in terms of a generalized perturbative expansion (resurgent expansion). Modified Bohr–Sommerfeld quantization conditions lead to generalized perturbative expansions which may be expressed in terms of nonanalytic factors of the form $\exp(-a/g)$, where $a > 0$ is the instanton action, and power series in the coupling g , as well as logarithmic factors. The ground-state energy, for the specific Hamiltonians, is shown to be dominated by instanton effects, and we provide numerical evidence for the validity of the related conjectures.

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1. Introduction

A number of intriguing and rather subtle issues are connected with simple Rayleigh–Schrödinger perturbation theory when it is applied to certain classes

of one-dimensional quantum mechanical model problems, which give rise to divergent perturbation series and allow for the presence of instanton effects [1]. Of particular interest is the case of the symmetric double-well potential [2,3]

$$\tilde{V}_{\text{dw}}(g, q) = \frac{1}{2}q^2(1 - \sqrt{g}q)^2, \quad (1)$$

E-mail addresses: jentschura@physik.uni-freiburg.de
(U.D. Jentschura), zinn@spht.saclay.cea.fr (J. Zinn-Justin).

the Hamiltonian being

$$\bar{H}_{\text{dw}} = -\frac{1}{2} \left(\frac{d}{dq} \right)^2 + \bar{V}_{\text{dw}}(g, q).$$

There are several points to note: (i) The perturbation series can be shown to be non-Borel summable [2,3] for positive g . (ii) The parity operation $q \rightarrow 1 - q$ leaves $\bar{V}_{\text{dw}}(g, q/\sqrt{g})$ invariant, and eigenfunctions are classified according to a principal quantum number N and the parity eigenvalue $\varepsilon = \pm$. States with the same principal quantum number but opposite parity are described by the same perturbative expansion. (iii) The energy splitting between states of opposite parity is described by nonanalytic factors of the form $\exp[-1/(6g)]$. In general, quantum tunneling may generate additional contributions to eigenvalues of order $\exp(-\text{const}/g)$, which have to be added to the perturbative expansion (for a review and more detail about barrier penetration in the semi-classical limit see, for example, [4]). Dominant contributions to the Euclidean path integral are generated by classical configurations (trajectories) that describe quantum mechanical tunneling among the two degenerate minima; their Euclidean action remains finite in the limit of large positive and large negative imaginary time (for a review see [5]).

Thus, the determination of eigenvalues starting from their expansion for small g is a non-trivial problem. Conjectures [6–10] have been discussed in the literature which give a systematic procedure to calculate eigenvalues, for finite g , from expansions which are shown to contain powers of the quantities g , $\ln g$ and $\exp(-\text{const}/g)$, i.e., resurgent [11,12] expansions. Moreover, generalized Bohr–Sommerfeld formulae (see, e.g., [13, Eq. (2)]) can be extracted by suitable transformations from the corresponding WKB expansions. (The approximate quantization conditions may also be derived from an exact evaluation of the path integral in the limit of a vanishing instanton interaction, by taking into account an arbitrary number of tunnelings between the minima of the potential [14–16].) Note that the relation to the WKB expansion is not completely trivial. Indeed, the perturbative expansion corresponds (from the point of view of a semi-classical approximation) to a situation with confluent singularities and thus, for example, the WKB expressions for barrier penetration are not uniform when the energy goes to zero.

Here, we are concerned with a modification of the double-well problem,

$$\bar{V}_{\text{FP}}(g, q) = \frac{1}{2} q^2 (1 - \sqrt{g} q)^2 + \sqrt{g} q - \frac{1}{2}, \quad (2)$$

the Hamiltonian being $\bar{H}_{\text{FP}} = -\frac{1}{2} (d/dq)^2 + \bar{V}_{\text{FP}}(g, q)$. The potential $\bar{V}_{\text{FP}}(g, q)$ also contains a linear symmetry-breaking term. There are the following points to note with regard to $\bar{V}_{\text{FP}}(g, q)$: (i) parity is not conserved, and there is no degeneracy of the spectrum on the level of the perturbative expansion. (ii) The perturbation series for the ground state vanishes identically to all orders in the coupling g [17]. (iii) The true ground-state energy is positive; in [17] it was shown that it fulfills $0 < E_0 < C \exp(-D/g)$, where C and D are positive constants. Here, we present a resurgent expansion which naturally leads to a generalization of perturbation theory valid for problematic potentials such as $\bar{V}_{\text{FP}}(g, q)$. Furthermore, we conjecture that a complete description of the energy eigenvalues can be obtained via a generalized Bohr–Sommerfeld quantization condition which allows for the presence of nonanalytic contributions of order $\exp[-1/(3g)]$ for the ground state and of order $\exp[-1/(6g)]$ for excited states, and we present numerical evidence for the validity of this conjecture. We thereby attempt to provide a complete description of the eigenvalues of the Fokker–Planck potential by a generalized perturbation series involving instanton contributions. More general cases are treated in [15,16].

We are not concerned here with supersymmetric quantum mechanics. In this context, the Fokker–Planck Hamiltonian has received some attention in the past two decades (see, e.g., [18,19]). Instead, we rather attempt to find the suitable generalization of perturbation theory that gives us an exact generalized secular equation for the energy eigenvalues which in turn yields a generalization of perturbation theory suitable to the problem at hand. We will not satisfy ourselves with an approximate solution of the problem but we attempt to find complete expressions for the energy eigenvalues in terms of resurgent expansions.

2. Fokker–Planck Hamiltonian

The particularly interesting Hamiltonian $\bar{V}_{\text{FP}}(g, q)$ has been studied in [17]. The spectra of the Hamil-

tonians \bar{H}_{dw} and \bar{H}_{FP} are invariant under the scale transformation $q \rightarrow q/\sqrt{g}$ and can therefore be written alternatively as

$$H_{\text{dw}} = -\frac{g}{2} \left(\frac{d}{dq} \right)^2 + \frac{1}{g} V_{\text{dw}}(q), \quad (3a)$$

$$V_{\text{dw}}(q) = \frac{1}{2} q^2 (1-q)^2, \quad (3b)$$

$$H_{\text{FP}} = -\frac{g}{2} \left(\frac{d}{dq} \right)^2 + \frac{1}{g} V_{\text{FP}}(q), \quad (3c)$$

$$V_{\text{FP}}(q) = V_{\text{dw}}(q) + g \left(q - \frac{1}{2} \right). \quad (3d)$$

This is a representation which illustrates that g takes the formal role of \hbar and that the linear symmetry-breaking term in $V_{\text{FP}}(q)$ in fact represents an explicit correction to the potential of relative order g .

For the double-well potential, the following two functions enter into the generalized Bohr–Sommerfeld quantization formula [9,13,14],

$$B_{\text{dw}}(E, g) = E + g \left(3E^2 + \frac{1}{4} \right) + g^2 \left(35E^3 + \frac{25}{4} E \right) + \mathcal{O}(g^3), \quad (4a)$$

$$A_{\text{dw}}(E, g) = \frac{1}{3g} + g \left(17E^2 + \frac{19}{12} \right) + g^2 \left(227E^3 + \frac{187}{4} E \right) + \mathcal{O}(g^3). \quad (4b)$$

The quantization condition and the resurgent expansion for the eigenvalues read:

$$\frac{1}{\sqrt{2\pi}} \Gamma \left(\frac{1}{2} - B_{\text{dw}}(E, g) \right) \left(-\frac{2}{g} \right)^{B_{\text{dw}}(E, g)} \times \exp \left[-\frac{A_{\text{dw}}(E, g)}{2} \right] = \varepsilon i, \quad (5)$$

and

$$E_{\varepsilon, N}(g) = \sum_{l=0}^{\infty} E_{N, l}^{(0)} g^l + \sum_{n=1}^{\infty} \left(\frac{2}{g} \right)^{Nn} \left(-\varepsilon \frac{e^{-1/6g}}{\sqrt{\pi g}} \right)^n \times \sum_{k=0}^{n-1} \left\{ \ln \left(-\frac{2}{g} \right) \right\}^k \sum_{l=0}^{\infty} e_{N, nkl} g^l. \quad (6)$$

Here, the $E_{N, l}^{(0)}$ are perturbative coefficients [6], and the expression for $E_{\varepsilon, N}(g)$ follows naturally from an expansion of (5) in powers of g , $\ln(g)$, and $\exp[-1/(6g)]$. The index n characterizes the order of the instanton contribution ($n = 1$ is a one-instanton, etc.). The conjecture (5) has been verified numerically to high accuracy [13].

Insight can be gained into the problem by considering the logarithmic derivative $S(q) = -g\psi'(q)/\psi(q)$, which for a general potential V satisfies the Riccati equation

$$gS'(q) - S^2(q) + 2V(q) - 2gE = 0. \quad (7)$$

This equation formally allows for solution with $E = 0$ (and implies a vanishing perturbation series), if the potential $V(q)$ has the following structure:

$$V(q) = \frac{1}{2} [U^2(q) - gU'(q)]. \quad (8)$$

Indeed, a formal solution of $H\phi = 0$ in this case is given by

$$\phi(q) = \exp \left[-\frac{1}{g} \int^q dq' U(q') \right]. \quad (9)$$

The Hamiltonian V_{FP} is of this structure, with $U(q) = U_{\text{FP}}(q) = q(1-q)$. This fact leads to the peculiar properties of V_{FP} , and indeed the Hamiltonians discussed in [17] belong to this class. The intriguing questions raised by the remarks made in [17] find a natural explanation in terms of generalized Bohr–Sommerfeld quantization conditions, and resurgent expansions.

Before discussing V_{FP} , we first make a slight detour and consider the special case $U_{\text{II}}(q) = q^3 + q$. The potential $\frac{1}{2}U_{\text{II}}^2(q)$ has no degenerate minima, and thus there are no instantons to consider. Indeed, in the case of the Hamiltonian $H_{\text{II}} = -(g/2)(d/dq)^2 + [U_{\text{II}}^2(q) - gU'_{\text{II}}(q)]/(2g)$ (we follow the notation of [17]), the expression (9) may be utilized for the construction of a normalizable eigenfunction of the Hamiltonian which reads $\phi_{\text{II}}(q) = \exp[-(q^2/2 + q^4/4)/g]$ and has the eigenvalue $E = 0$.

In the case of the potential $U_{\text{FP}}(q) = q(1-q)$, the issue is more complicated because the wave function

$$\phi(q) = \exp \left[\frac{1}{g} \left(\frac{q^3}{3} - \frac{q^2}{2} \right) \right] \quad (10)$$

is not normalizable, and thus is not an eigenfunction. An analogy of the Riccati equation (7) with the Fokker–Planck equation suggests that the case $E = 0$ be identified with an equilibrium probability distribution. Therefore, the non-normalizable wave function (10) may naturally be identified with a “pseudo-equilibrium” distribution.

3. Instanton action

The Euclidean instanton action for the ground state of the Fokker–Planck potential is given by [8,9]

$$a = 2 \int_0^1 dq U_{\text{FP}}(q) = \frac{1}{3}, \quad (11)$$

and it is this quantity which determines the leading contribution to the ground-state energy of order $\exp[-1/(3g)]$. We conjecture here the following generalized quantization condition for the eigenvalues of the Hamiltonian (3c)

$$\frac{1}{\Gamma t(-B_{\text{FP}}(E, g))\Gamma(1 - B_{\text{FP}}(E, g))} + \left(-\frac{2}{g}\right)^{2B_{\text{FP}}(E, g)} \frac{\exp(-A_{\text{FP}}(E, g))}{2\pi} = 0. \quad (12)$$

This condition is different from what would be obtained if one were to consider perturbation theory alone. Indeed, the perturbative quantization condition reads

$$B_{\text{FP}}(E, g) = N, \quad (13)$$

with integer $N \geq 0$. The functions B_{FP} and A_{FP} determine the perturbative expansion, and the perturbative expansion about the instantons, in higher order. They have the following expansions:

$$\begin{aligned} B_{\text{FP}}(E, g) &= E + 3E^2g + \left(35E^3 + \frac{5}{2}E\right)g^2 \\ &+ \left(\frac{1155}{2}E^4 + 105E^2\right)g^3 \\ &+ \left(\frac{45045}{4}E^5 + \frac{15015}{4}E^3 + \frac{1155}{8}E\right)g^4 \end{aligned}$$

$$\begin{aligned} &+ \left(\frac{969969}{4}E^6 + \frac{255255}{2}E^4 + \frac{111111}{8}E^2\right)g^5 \\ &+ \left(\frac{22309287}{4}E^7 + \frac{33948915}{8}E^5\right. \\ &+ \left.\frac{3556553}{4}E^3 + \frac{425425}{16}E\right)g^6, \\ &+ \left(\frac{2151252675}{16}E^8 + \frac{557732175}{4}E^6\right. \\ &+ \left.\frac{379257879}{8}E^4 + 4157010E^2\right)g^7 + \mathcal{O}(g^8), \end{aligned} \quad (14a)$$

$$\begin{aligned} A_{\text{FP}}(E, g) &= \frac{1}{3g} + \left(17E^2 + \frac{5}{6}\right)g \\ &+ \left(227E^3 + \frac{55}{2}E\right)g^2 \\ &+ \left(\frac{47431}{12}E^4 + \frac{11485}{12}E^2 + \frac{1105}{72}\right)g^3 \\ &+ \left(\frac{317629}{4}E^5 + \frac{64535}{2}E^3 + \frac{4109}{2}E\right)g^4 \\ &+ \left(\frac{26145967}{15}E^6 + \frac{25643695}{24}E^4\right. \\ &+ \left.\frac{4565723}{30}E^2 + \frac{82825}{48}\right)g^5 \\ &+ \left(\frac{812725953}{20}E^7 + \frac{280162805}{8}E^5\right. \\ &+ \left.\frac{1057433447}{120}E^3 + \frac{20613005}{48}E\right)g^6 + \mathcal{O}(g^7). \end{aligned} \quad (14b)$$

The calculation of A - and B -functions, for general classes of potentials, is described in more detail in [15, 16]. On the basis of (13) and (14a), we obtain the following perturbative expansion $E_N^{(\text{pert})}(g)$ up to and including terms of order g^3 , for general N ,

$$\begin{aligned} E_N^{(\text{pert})}(g) &\sim N - 3N^2g - \left(17N^3 + \frac{5}{2}N\right)g^2 \\ &- \left(\frac{375}{2}N^4 + \frac{165}{2}N^2\right)g^3 + \mathcal{O}(g^4). \end{aligned} \quad (15)$$

Here, the upper index (0) means that only the perturbative expansion (in powers of g) is taken into account. For the ground state ($N = 0$), all the terms vanish,

whereas for excited states with $N = 1, 2, \dots$, the perturbation series is manifestly nonvanishing.

The quantization condition (12) is conjectured to be the secular equation whose solutions determine the energy eigenvalues of the Fokker–Planck potential (3d). Eqs. (14a) and (14b) can be used to expand the ground-state energy eigenvalue up to sixth order in the nonperturbative factor $\exp(-1/3g)$, and up to seventh order in the coupling g . The general structure of the resurgent expansions determined by (12) differs slightly for the ground state in comparison to the excited states. This will be shown below, with a special emphasis on the ground state.

4. Resurgent expansion for the ground state

Based on (12), we derive the following expansion for the ground-state energy ($N = 0$) of the Fokker–Planck potential (3d):

$$E_{\text{FP}}^{(0)}(g) = \sum_{n=1}^{\infty} \left(\frac{e^{-1/3g}}{2\pi} \right)^n \sum_{k=0}^{n-1} \left\{ \ln \left(-\frac{2}{g} \right) \right\}^k \times \sum_{l=0}^{\infty} f_{nkl}^{(0)} g^l. \quad (16)$$

For small coupling g , this expansion is strongly dominated by the one-instanton effect ($n = 1$). An explicit calculation using (14a) and (14b) leads to the following expansion for the ground-state energy of the Hamiltonian H_{FP} , which is valid up to terms of order $[\exp(-1/3g)]^2$,

$$E_{\text{FP}}^{(0)}(g) \sim \frac{\exp(-\frac{1}{3g})}{2\pi} \left(1 - \frac{5}{6}g - \frac{155}{72}g^2 - \frac{17315}{1296}g^3 - \frac{3924815}{31104}g^4 - \frac{3924815}{31104}g^4 - \frac{294332125}{186624}g^5 - \frac{163968231175}{6718464}g^6 - \frac{18124314587725}{40310784}g^7 - \frac{18587546509880725}{1934917632}g^8 + \mathcal{O}(g^9) \right) + \mathcal{O}([\exp(-1/3g)]^2). \quad (17)$$

Because the perturbation series (15) vanishes for $N = 0$, the resurgent expansion starts with the one-

instanton effect. Indeed, Eq. (17) is the one-instanton contribution to the energy, characterized by a non-analytic factor $\exp(-1/3g)$ which is multiplied by a (divergent, nonalternating) power series in g . This nonalternating series in g may be resummed by a generalized Borel method (the generalized Borel sum finds a natural representation in the sense of distributional Borel summability, which is effectively a Borel sum in complex directions of the parameters, see, e.g., [20–24]).

In analogy to the double-well potential, the imaginary part which is generated by this procedure (the “discontinuity” of the distributional Borel sum in the terminology of [22]) is compensated by an explicit imaginary part that originates from the two-instanton effect. We supplement here the first few terms of the two-instanton shift of the ground-state eigenvalue (terms with $n = 2$ in Eq. (16)):

$$\frac{[\exp(-1/3g)]^2}{(2\pi)^2} \left\{ 2 \ln \left(-\frac{2}{g} \right) + 2\gamma + g \left[-\frac{10}{3} \ln \left(-\frac{2}{g} \right) - \frac{10}{3} \gamma - 3 \right] + \mathcal{O}(g^2 \ln g) \right\}. \quad (18)$$

Here, $\gamma = 0.577216\dots$ is Euler’s constant.

The perturbative coefficients about one instanton, called $f_{10K}^{(0)}$ in Eq. (16), grow factorially as

$$f_{10K}^{(0)} \sim -\frac{3^K \Gamma(K)}{\pi}, \quad K \rightarrow \infty. \quad (19)$$

It is an easy exercise to verify that this factorial growth exactly leads to an imaginary part that is canceled by the imaginary part that results from the analytic continuation of the expression $2 \ln(-2/g) + 2\gamma$ in (18) from negative to positive g . The explicit coefficients in (17) are consistent with the asymptotic formula (19).

We have performed extensive numerical checks on the validity of the expansion (17). For example, at $g = 0.007$, the ground-state energy, obtained numerically, is

$$E_{\text{FP}}^{(0)}(0.007) = 3.300\,209\,301\,936(1) \times 10^{-22} \quad (20)$$

based on a calculation with a basis set composed of up to 300 harmonic oscillator eigenstates. The numerical uncertainty is estimated on the basis of the apparent

convergence of the results under an appropriate increase of the number of states in the basis set.

When adding all terms up to the order of g^9 in the perturbative expansion about the leading instanton (the first eight terms are given in Eq. (17), further terms are available for download [25]), we obtain

$$E_{\text{FP}}^{(0)}(0.007) \approx 3.300\,209\,301\,942 \times 10^{-22}. \quad (21)$$

With the term of order g^{10} included, we have

$$E_{\text{FP}}^{(0)}(0.007) \approx 3.300\,209\,301\,936 \times 10^{-22} \quad (22)$$

in full agreement with (20) to all decimals shown.

We should clarify why the n -instanton contribution in the resurgent expansion (6) for the double-well potential (3b) involves the n th power of the expression $\exp(-1/6g)$, while in the case of the ground-state of the Fokker–Planck Hamiltonian it involves the n th power of $\exp(-1/3g)$. One may answer this question by observing that in a symmetric potential, instanton configurations with an odd number of tunnelings between the minima yield a nonvanishing contribution to the path integral, and therefore, the “one-instanton” configuration in the double-well is a trajectory that starts in one well and ends in the other. The linear symmetry-breaking term of the Fokker–Planck potential lifts this degeneracy; the leading, “one”-instanton shift of the ground state is now a configuration in which the particle returns to the well from which it started; the instanton action is therefore twice as large and the two-instanton contribution (the “bounce”-configuration in the case of the double-well potential) becomes the one-instanton solution in the case of the ground-state of the Fokker–Planck equation.

As a last remark, it is useful to observe that although the correction term $g(q - \frac{1}{2})$ in Eq. (3d) vanishes in the limit $g \rightarrow 0$, one cannot recover the double-well quantization condition (5) from (12) in this limit; it is nonuniform.

5. Resurgent expansion for excited states

The energy of excited states ($N > 0$) is dominated, for small g , by the perturbative expansion (15) which is manifestly nonvanishing to all orders in g . Because the symmetry is broken only at order g (see Eq. (3d)), and because the dominance of the perturbation series

(expansion in g) is fully restored for excited states, the resurgent expansion induced by (12) becomes very close to the analogous expansion for the states of the double-well potential (6). By direct expansion of (12), taking advantage of the functional form of the dependence of $A_{\text{FP}}(g)$ and $B_{\text{FP}}(g)$ on g , we obtain the resurgent expansion

$$E_{\text{FP}}^{(\varepsilon, N>0)}(g) = E_N^{(\text{pert})}(g) + \sum_{n=1}^{\infty} [-\varepsilon \mathcal{E}_N(g)]^n \sum_{k=0}^{n-1} \left\{ \ln\left(-\frac{2}{g}\right) \right\}^k \times \sum_{l=0}^{\infty} f_{nkl}^{(N)} g^l. \quad (23)$$

Here, $\varepsilon = \pm$ is a remnant of the parity which is broken by $V_{\text{FP}}(g)$, but only at order g , $E_N^{(\text{pert})}(g)$ is the perturbative expansion given in (15), and $\mathcal{E}_N(g)$ is given by

$$\mathcal{E}_N(g) = \sqrt{\frac{2}{\pi}} \frac{2^{N-1} \exp(-1/6g)}{g^N \sqrt{N!(N-1)!}}. \quad (24)$$

For completeness, we indicate here the first few terms for the resurgent expansion of the states with $N = 1$, but opposite (perturbatively broken) parity $\varepsilon = \pm$, to leading order in the coupling up to the three-instanton term,

$$E_{\text{FP}}^{(\pm, N=1)}(g) = 1 + \mathcal{O}(g) \mp \mathcal{E}_1(g)(1 + \mathcal{O}(g)) + [\mathcal{E}_1(g)]^2 \left[\ln\left(-\frac{2}{g}\right) + \gamma - \frac{1}{2} + \mathcal{O}(g \ln g) \right] \mp [\mathcal{E}_1(g)]^3 \left[\frac{3}{2} \ln^2\left(-\frac{2}{g}\right) + \left(-\frac{3}{2} + 3\gamma\right) \ln\left(-\frac{2}{g}\right) + \frac{5}{8} - \frac{3}{2}\gamma + \frac{3}{2}\gamma^2 + \frac{\pi^2}{12} + \mathcal{O}(g \ln g) \right]. \quad (25)$$

6. Conclusions

We have presented the quantization condition (12) which, together with Eqs. (14a) and (14b), determines the resurgent expansions for an arbitrary state (quantum number N) of the Fokker–Planck potential (3c) up

to seventh order in the coupling g , and up to and including the six-instanton order. For general $N > 0$, the perturbation series is nonvanishing (see Eq. (15)), and the instanton contributions, for small coupling, yield tiny corrections to the energy. However, for the ground state with $N = 0$, the perturbation series vanishes to all orders in the coupling, and the resurgent expansion (16) for the ground-state energy of the Fokker–Planck potential (3c) is dominated by the nonperturbative factor $\exp(-1/3g)$ that characterizes the one-instanton contribution to the ground-state energy. The nonperturbative factor $\exp(-1/3g)$ is multiplied by a factorially divergent series (see Eqs. (17) and (19)); this is the natural structure of a resurgent expansion which holds also for the double-well potential (see Eq. (6)). The basic features of this intriguing phenomenon have been described in [17]; they find a natural and complete explanation in terms of the resurgent expansions discussed here.

Concepts discussed in the current Letter may easily be generalized to more general symmetric potentials with degenerate minima, potentials with two equal minima but asymmetric wells, and periodic-cosine potentials (some further examples are discussed in [15,16]). There is a well-known analogy between a one-dimensional field theory and one-dimensional quantum mechanics, the one-dimensional field configurations being associated with the classical trajectory of the particle. Indeed, the loop expansion in field theory corresponds to the semi-classical expansion [26, Chapter 6]. Therefore, one might hope that suitable generalizations of the methods discussed here could result in new conjectures for problems where our present understanding is (even) more limited.

Resurgent expansions appear to be of wide applicability in a number of cases where ordinary perturbation theory, even if augmented by resummation prescriptions, fails to describe physical observables such as energy eigenvalues even qualitatively. This has been demonstrated here using the Fokker–Planck potential as an example.

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