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Discrepancies from Asymptotic Series and Their Relation to Complex Classical Trajectories

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There exist functions $F(x)$ whose asymptotic expansions, when computed at fixed x and optimal order, seem to converge to a numerical value which deviates significantly from $F(x)$ itself. Several examples are given, showing that this phenomenon is not exceptional, and should occur in quantum theory. In particular, the semiclassical expansion, at large quantum numbers, of levels of the quartic oscillator $V=x^4$ presents such discrepancies, which we explain quantitatively as contributions from classical trajectories for which space and time coordinates become complex.

When asymptotic expansions are used for practical purposes, the following procedure is currently followed: The sequence $F^{(k)}(x)$ of partial sums for the function $F(x)$ $(x\to\infty)$ is constructed for a large but *fixed* value of the variable x. The best estimate $F^*(x)$ is allegedly attained by stopping at the rank $k=K$ such the Kth term of the series is smallest. The value ϵ of this last term is assumed to provide an order of magnitude for the actual error $F(x)-F^*(x)$. Such a procedure does not rely on the mathematical definition of the asymptotic expansion (k fixed, $x\to\infty$), but rather on a faith supported by experience. If in some cases [such as the Stirling expansion of $\Gamma(x)$ for x real] it may be proven that $|F(x)-F^*(x)|<\epsilon$, nothing prevents in general the sequence $F^{(k)}(x)$ from exhibiting an extremely flat plateau of width ϵ around $F^*(x)$, while the exact value $F(x)$ lies elsewhere, at a distance from the plateau *much larger than* ϵ. The "best" estimate provided by the asymptotic expansion will then be quite unreliable.

As a first example, consider the asymptotic expansion of the Bessel function,

$$\pi(2\pi z)^{1/2}J_0(z)\approx e^{-i(z-\pi/4)}\sum_{k=0}^{\infty}\frac{[\Gamma(k+\frac{1}{2})]^2}{(-2iz)^k k!}+e^{i(z-\pi/4)}\sum_{k=0}^{\infty}\frac{[\Gamma(k+\frac{1}{2})]^2}{(2iz)^k k!},\qquad(1)$$

valid for z real and large. When $0<\arg z<\frac{1}{2}\pi$, for $|z|\to\infty$, the second part of this expansion decreases exponentially; from a mathematical point of view, it is negligible when compared with all terms of the first series, and should be dropped. For numerical purposes, however, it is quite significant, even if y, the imaginary part of $z=x+iy$, is large. For instance (see Fig. 1), the successive approximations for $J_0(5+3i)$ provided by the first part of the expansion (1) suggest that

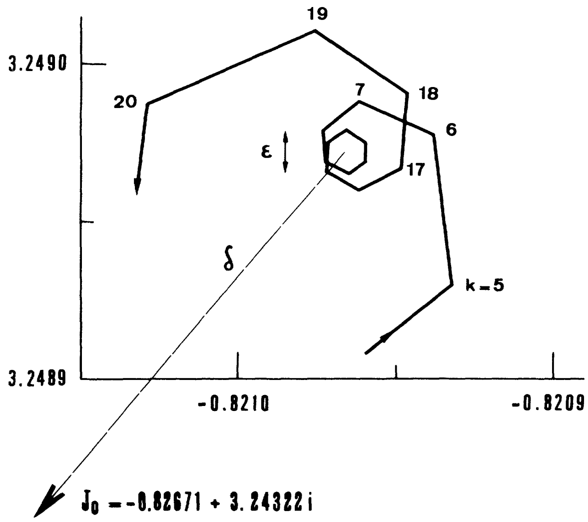

FIG. 1. Convergence in the complex plane of the asymptotic expansion of $J_0(5+3i)$.

the best estimate $J_0^* \simeq -0.82097+3.24987i$ ($K=12\pm3$) approaches J_0 within an error $\epsilon \simeq 10^{-5}$; however, a much larger discrepancy between J_0^* and J_0 exists, which is well accounted for by the exponentially small term $\delta \simeq (2\pi z)^{-1/2} e^{i(z-\pi/4)} \simeq -(5.7+5.9i)\times 10^{-3}$. For general z, the smallest term (of rank $K \sim |2z|$) yields for the best estimate an apparent uncertainty ϵ of magnitude $e^{-|2z|}$. However, the exponentially small correction δ in (1) has magnitude e^{-2y}, which is much larger than ϵ as long as $|\arg z| < \frac{1}{2}\pi$, and should be retained (except along the Stokes line[1] $\mathrm{Re}z=0$). Of course, this correction δ would be absent for Hankel functions.

Such results extend to asymptotic expansions generated by the method of steepest descent. Consider an integral along a complex path,

$$F(x)=\int e^{-x\varphi(u)}du, \qquad (2)$$

where $\varphi(u)$ is analytic, and assume for simplicity that one saddle point at $u=0$, with $\varphi(0)=0$ and $\varphi''(0)\neq 0$, dominates in the limit $x\to+\infty$. Subdominant saddles, at a lower altitude, may be crossed by the path, and give exponentially small contributions, which we intend to compare with the "error" ϵ, estimated naively as the smallest term of the asymptotic expansion

$$F(x)\sim\sum_{k=0}^{\infty}F_k x^{-k-1/2}.$$

This expansion is constructed by taking $i\varphi(u)=s$ as the integration variable, which transforms (2) into

$$F(x)=\int e^{ixs}\rho(s)\,ds. \qquad (3)$$

Since $\mathrm{Re}\varphi(u)\geq 0$ along the integration path of (2), the integration contour of (3) lies on the Riemann surface of $\rho(s)$ in the half-plane $\mathrm{Im}s\geq 0$, except that it makes a loop about the branch point $s=0$ which corresponds to the dominant saddle point $u=0$. By making the expansion

$$\rho(s)=\sum_{n=-1}^{\infty}\rho_{n/2}s^{n/2},$$

we find that the coefficients of the expansion of $F(x)$ are

$$F_k=2i^{k+1/2}\Gamma(k+\tfrac{1}{2})\rho_{k-1/2}.$$

Thus, the behavior of F_k for k large is governed by the radius of convergence $|s_\epsilon|$ of the series

$$\rho_{\mathrm{odd}}(s)=\sum_{k=0}^{\infty}\rho_{k-1/2}s^{k-1/2}.$$

Here s_ϵ is the singularity of $\rho(s)$ closest to the origin and lying on either of the two sheets associated with the branch point $s=0$. By standard techniques[2] we then find that for x large and fixed, the smallest term of the asymptotic series, of rank $K\sim x|s_\epsilon|$, has size $\epsilon \propto \exp(-x|s_\epsilon|)$. On the other hand, in order to exhibit the contribution to $F(x)$ of subdominant saddles, if any, one should push the integration contour of (3) upwards, as far as is allowed by the singularities of $\rho(s)$. Then the *lowest* singularity s_δ encountered by the contour besides $s=0$ yields a contribution δ to $F(x)$ proportional to $\exp(ixs_\delta)$ in the limit of large x. This contribution, although exponentially small since $\mathrm{Im}s_\delta>0$, is nonetheless relevant if it dominates ϵ. Two generic situations occur:

(i) $|s_\epsilon| < Ims_\delta$.—The contributions from subdominant saddles, if any, are negligible, and the asymptotic expansion is reliable within an error of order ϵ. Examples include the function $\Gamma(x)$ and the Hankel functions ($s_\delta=i\infty$), and more generally any function equal to the Borel sum of its asymptotic expansion.

(ii) $|s_\epsilon| > Ims_\delta$.—A systematic deviation is then introduced by the asymptotic expansion, which should be corrected by including the contribution from the subdominant saddle. Such a contribution is relevant even in the limit $x\to\infty$, since $|\delta/\epsilon|\to\infty$. An example is the integral (2) taken on the real axis with $\varphi(u)=36u^2-20u^3+3u^4$: The subdominant saddle point is $u=3$ ($s_\delta=27i$), whereas the saddle point $u=2$ ($s_\epsilon=32i$) controls the behavior of the asymptotic expansion. Another example is the Bessel function $J_0(z)$ ($\mathrm{Re}\, z > 0$) seen above, for which $s_\epsilon = s_\delta$ but $\delta \gg \epsilon$.

The semiclassical expansions of quantum mechanics (and the perturbation expansions of field theory) present some analogy with asymptotic expansions generated by a path integral, since Feynman integrals from which they may be derived look like (2): x is replaced by $1/\hbar$ (or by the inverse coupling constant), the integration variable u by the trajectories in configuration space, and $i\varphi(u)$ by the action along such a trajectory. For analytic potentials, the function $\rho(s)$ which arises as in (3) when taking the action as a variable is expected to be analytic. When the integration contour on s (real axis) is pushed upwards, a dominant contribution arises from each singularity of $\rho(s)$ on the real axis, i.e., from each classical trajectory which makes the action stationary; the semiclassical expansion results by expanding $\rho(s)$ around these real singularities. However, subdominant contributions δ are expected to arise, as above, from singularities s_δ of $\rho(s)$ in the upper half-plane, i.e., *from complex classical trajectories*,[3] solutions of the classical equations of motion for complex space and time variables (or for complex field variables). Here again, δ may dominate the smallest terms of the asymptotic expansion in powers of $\hbar$. It is then pertinent, while using a semiclassical expansion (or a perturbation expansion in field theory), to take into account the complex trajectories whose actions have small imaginary parts.

Let us illustrate this qualitative idea by studying the energy levels E_n of the quartic oscillator $H = p^2 + x^4$ (setting $\hbar = 2m = 1$). Numerical calculations[4] exhibit a good "convergence" for the semiclassical estimates $E_n^{(k)}$ of E_n in inverse powers of the quantum number n, which are obtained by solving equations of the form

$$(n+\tfrac{1}{2})\pi = \sigma + \sum_{j=1}^{*k} b_j \sigma^{-2j+1}, \tag{4}$$

$$\sigma \equiv \int_{-E^{1/4}}^{E^{1/4}} (E - x^4)^{1/2}\, dx = E^{3/4}[\Gamma(\tfrac{1}{4})]^2/[3(2\pi)^{1/2}]. \tag{5}$$

The first eight terms of the series (4) have been given by Bender, Olaussen, and Wang[4] ($b_1 = -\frac{1}{12}\pi$, $b_2 = 11[\Gamma(\frac{1}{4})]^2\pi^2/165\,888, \ldots$). By their method, we have obtained b_j up to $j = 16$ in closed form, and up to $j = 53$ numerically. Large-order terms fit well with the following asymptotic expression of b_j:

$$b_j \underset{j\to\infty}{\sim} \Gamma(2j-1)2^{-j\pm 3/2}\pi^{-1}\sin(\tfrac{1}{2}j\pi - \tfrac{3}{4}\pi)\left(1 + \frac{\alpha_1}{2j-2} + \frac{\alpha_2}{(2j-2)(2j-3)} + \cdots\right), \tag{6}$$

where α_l is given in terms of the b_k ($2k < l+2$) by

$$1 + \sum_{l=1}^{\infty} \alpha_l \sigma^{-1} \equiv \exp(2b_1\sigma^{-1} + 4b_2\sigma^{-3} - 8b_3\sigma^{-5} - 16b_4\sigma^{-7} + \cdots) \tag{6'}$$

($\alpha_1 = -\pi/6$, $\alpha_2 = \pi^2/72, \ldots$). Equations (6) and (6′) have been derived through a semiclassical analysis of the Borel transform[2] of the series (4).

The quantization rule (4) relies on real closed trajectories, bouncing between the real turning points $x = \pm E^{1/4}$, and on small fluctuations around them. But this semiclassical expansion is again plagued by a systematic discrepancy (Table I), which we explain by the existence of complex closed trajectories, making loops on the Riemann surface (Fig. 2) of the complex action $S(z) = \int_0^z (E - x^4)^{1/2}\, dx$, around any of the four turning points satisfying $x^4 = E$. The corresponding values of the action $s = p\sigma + iq\sigma$ ($p+q$ even) are the singularities of the function $\rho(s)$ of (3). According to the above analysis, the "convergence" of semiclassical expansions is governed by the complex singularities s_ϵ lying closest to the dominant ones $s_0 = 2p\sigma$, i.e., $s_\epsilon = (2p+1)\sigma \pm i\sigma$, with $|s_\epsilon - s_0| = \sigma\sqrt{2}$ [these singu-

TABLE I. Semiclassical estimates for a sample of energy levels of the quartic oscillator. The "best" estimates E_n^* differ significantly from the exact values E_n. Deviations are explained by the contribution δ from complex classical trajectories [Eq. (8)].

	$n=0$	$n=3$	$n=6$
$E_n^{(0)}$	0.87[a]	11.611 525 3	26.506 335 510 963
$E_n^{(1)}$	0.98[a]	11.644 989 5	26.528 512 551 757
$E_n^{(3)}$	0.79	11.644 765 8	26.528 471 147 158
$E_n^{(5)}$	1.40	11.644 768 2	26.528 471 181 652
$E_n^{(7)}$		11.644 767 9[a]	26.528 471 181 390
$E_n^{(9)}$		11.644 768 1[a]	26.528 471 181 401[a]
$E_n^{(11)}$		11.644 767 9	26.528 471 181 399[a]
δ	0.15	−0.000 023 6	0.000 000 002 343
$E_n^* + \delta$	1.07	11.644 744 4	26.528 471 183 742
E_n	1.060	11.644 745 51	26.528 471 183 682

[a]Values from which the "best" estimate E_n^* (for a given quantum number n) is made.

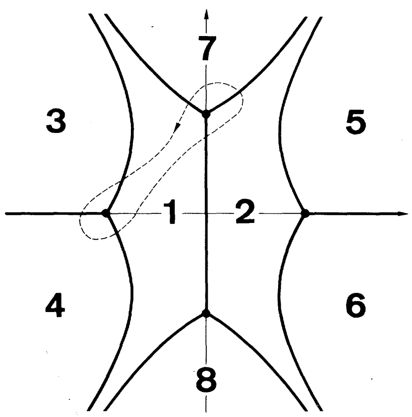

FIG. 2. The plane of complex coordinates x for the potential $V=x^4$. The asymptotic expression of the wave function is discontinuous along the Stokes lines (heavy solid lines), issuing from the two real and the two imaginary turning points. The dashed line shows a complex classical trajectory tunneling from a real to an imaginary turning point.

larities are precisely responsible for the asymptotic expansion (6)]. Accordingly, the apparent accuracy of semiclassical expansions is $\epsilon \propto \exp\{-\sigma\sqrt{2}/\hbar\}$. However, the complex trajectories associated with the lowest-lying singularities $s_\delta=(2p+1)\sigma+i\sigma$ also yield subdominant contributions, proportional to $\delta \propto \exp\{-\sigma/\hbar\}$. We are thus in case (ii): Complex trajectories contribute significantly even in the semiclassical limit.

More precisely, let us calculate the resulting correction δ for the nth energy level E_n, to lowest order: We shall systematically retain terms in $e^{-\sigma/\hbar}$, but drop power terms in $\hbar/\sigma$. In each of the regions $\alpha=1, 2, \ldots, 8$ of the complex x plane limited by the Stokes lines (Fig. 2), the eigenfunction is then represented by an approximation $(E-x^4)^{-1/4}[A_\alpha e^{iS/\hbar}+B_\alpha e^{-iS/\hbar}]$. The WKB matching procedure connects the values of the constants A and B from one region to the other, in particular around the turning points $\pm iE^{1/4}$, for which[5] $A_2=A_1(1+e^{-2\sigma})^{1/2}-iB_1e^{-\sigma}$ and $B_2=iA_1e^{-\sigma}+B_1(1+e^{-2\sigma})^{1/2}$ (we have reset $\hbar=1$). The boundary conditions $A_3=B_4=A_5=B_6=0$ provide the quantization rule, which comes out as $(1+e^{-2\sigma})^{1/2}\cos\sigma+e^{-\sigma}=0$, or equivalently as

$$(n+\tfrac{1}{2})\pi=\sigma-(-1)^n\arctan e^{-\sigma}. \qquad (7)$$

Together with (5), this equation yields the subdominant contribution δ to the energy levels E_n. To lowest order in $e^{-\sigma}$ and $1/\sigma$,

$$\delta \simeq (-1)^n \tfrac{4}{3}E_n \exp[-(n+\tfrac{1}{2})\pi]/(n+\tfrac{1}{2})\pi \qquad (8)$$

explains indeed most of the discrepancy between the best estimate $E_n{}^*$ and the exact value E_n (Table I).

If we now consider the potential $V=x^4+ax$, and let a increase, the topology of the Stokes lines changes: When $a=a_0\simeq 1.18E^{3/4}$, the two complex turning points enter regions 5 and 6 of Fig. 2 and become inactive[6]; the subdominant correction δ disappears for $a>a_0$.

Thus, subdominant contributions from complex solutions of the classical equations of motion may provide corrections which, although small as $\exp\{-\mathrm{Im}\,s_\delta/\hbar\}$, are numerically relevant. Since the idea of considering complex classical trajectories for evaluating quantum effects is popular in the theory of heavy-ion nuclear collisions,[6,7] the above remarks may help us to understand the practical success of such methods. In quantum field theory, solutions of the complex classical field equations, namely instantons,[2] are also currently used, both in the study of the tunneling effect and to get nonperturbative information from the large orders of perturbation series. The present analysis suggests using them further to add subdominant corrections to the perturbation expansions.

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