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Higher-Order Variational Approach to Non-Borel Systems. The Energies of the Double-Well Potential

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May 3, 1994

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Abstract

The recently proposed improvement scheme for the effective classical potential is applied to a system whose perturbation expansion is of the non-Borel type: the double-well potential. The expansion is found to converge fast everywhere from low couplings, where level splitting has to be included, to strong coupling, where the asymptotic behavior is well reproduced.

Some time ago, Feynman and the author [1] presented a variational approach by which a path integral is converted into an ordinary integral over a Boltzmann factor involving an effective classical potential

$$Z = \int \frac{dx_0}{\sqrt{2\pi\hbar\beta/M}} e^{-\beta V^{\text{eff}}_{\text{cl}}(x_0)}, \quad (1)$$

where x_0 is the temporal path average $x_0 = \int_0^{\hbar} d\tau x(\tau)$. The reason for the separate treatment of x_0 is that the fluctuations around x_0 are small at all temperatures and can be treated approximately. This is in contrast to the violent fluctuations of x_0 itself at increasing temperatures which, in general, do not permit any approximation and must be integrated numerically in (1). The approach produces quite good estimates for the free energy and particle distributions of a wide variety of quantum systems [2]. An approximation to the usual effective potential can be calculated which, in contrast to traditional loop expansions, is automatically convex even at lowest order [3].

The approach has been developed further by the author into a systematic expansion which converges rapidly towards the correct result [4], [5] (see also [6]). The observed convergence of the expansion scheme has not yet been proven mathematically. This should, however, be possible by an appropriate adaptation of presently available proofs for asymptotic expansions of the anharmonic integral [7]. The convergence is caused by a similar mechanism that leads to convergent resummations via order-dependent mapping techniques [8].

Recently, a variational approach has also been found for the regime of negative coupling constant g [9], where the partition function has a cut with an imaginary part proportional to $|g|^b e^{-1/a|g|}$. There exists now a rapidly convergent expansion scheme for calculating this imaginary part which produces very accurate results over the entire left-hand cut [10]. The accuracy is so high that a dispersion relation in the complex g -plane reproduces very well the energies at positive g . Its power series expansion yields the perturbation coefficients starting from the tailend of the series—which is governed by the well-known semiclassical approximation to tunneling—and continuing down to lowest order. One may call this a *backward perturbation expansion* [12].

The purpose of this note is to show that also notorious non-Borel summable systems [11] can be treated with variational methods. As a typical

example we consider the double-well potential

$$V(x) = \omega^2 x^2/2 + gx^4/4, \quad \omega^2 = -1 \quad (2)$$

and calculate the lowest two energies at arbitrary coupling g . The results agree well with numeric solutions of the Schrödinger equation.

The effective classical potential $V^{\text{eff-cl}}(x_0)$ of the double-well potential is obtained in three steps (for details see [4], [5]):

i) Expand $V(x)$ around x_0 in powers of $\delta x \equiv x - x_0$:

$$V(x) = V(x_0) + V'(x_0)(\delta x) + \frac{1}{2}V''(x_0)(\delta x)^2 + \dots \quad (3)$$

ii) Set up a diagrammatic perturbation expansion for the effective energy at a fixed x_0 up to the order N in the coupling $g_3(x_0) \equiv V'''(x_0)$, $g_4(x_0) \equiv V^{(iv)}(x_0), \dots$. The lines in the diagrams represent the correlation function $\langle \delta x(\tau) \delta x(0) \rangle$ whose Fourier transform equals that of a harmonic oscillator, except for the absence of the zero-frequency Matsubara mode:

$$\begin{aligned} G(\tau) &= \frac{2}{\hbar\beta} \sum_{m=1}^{\infty} \frac{1}{\omega_m^2 + \omega^2} e^{i\omega\tau} \\ &= \frac{1}{\omega} \frac{\cosh[(\hbar\beta - \tau)\omega/2]}{\sinh[\hbar\beta\omega/2]} - \frac{1}{\beta\omega}. \end{aligned} \quad (4)$$

Due to this property, tadpole diagrams disappear by energy conservation.

iii) Replace ω everywhere by $\sqrt{\Omega^2(x_0) + g_2(x_0)}$ where $g_2(x_0) \equiv V''(x_0)$, $\Omega^2(x_0)$ is the quadratic vertex ("local mass term"), expand the square root in powers of $g_2(x_0)$ and collect all terms up to the order N in the couplings g_i .

iv) Extremize the resulting function $W_N(x_0)$ in $\Omega(x_0)$ for each value of x_0 .

For the anharmonic oscillator, the diagrammatic expansion is up to third order

$$W_3(x_0) = V(x_0) + \frac{1}{\beta} \left\{ -\frac{1}{2} \bigcirc + \left(\frac{1}{2} \bigcirc + \frac{1}{8} \bigcirc \bigcirc \right) \right\}$$

$$\begin{aligned}
& -\frac{1}{2} \left[\frac{1}{2} \text{ (circle) } - \frac{1}{2} \text{ (two circles) } + \frac{1}{6} \text{ (horizontal ellipse) } + \frac{1}{24} \text{ (vertical ellipse) } + \frac{1}{8} \text{ (three circles) } \right] \\
& + \frac{1}{6} \left[\text{ (large circle) } + \frac{3}{2} \text{ (horizontal ellipse) } + 3 \left(\frac{1}{4} \text{ (two circles) } + \frac{1}{2} \text{ (three circles) } \right) \right. \\
& \quad + 3 \left(\frac{1}{4} \text{ (two circles with top loop) } + \frac{1}{4} \text{ (triangle in circle) } \right) \\
& \quad + 3 \left(\frac{1}{4} \text{ (three circles) } + \frac{1}{6} \text{ (vertical ellipse) } + \frac{1}{4} \text{ (four circles) } \right) \\
& \quad \left. + \left(\frac{3}{16} \text{ (four circles) } + \frac{1}{4} \text{ (horizontal ellipse with top loop) } + \frac{1}{8} \text{ (triangle in circle) } + \frac{1}{8} \text{ (four circles with top loop) } \right) \right] \Bigg\}.
\end{aligned}$$

For the analytic expressions of the diagrams see the forthcoming second edition of [2]. The energies obtained after extremizing $W_3(x_0)$ are plotted in Fig. 1 where they are compared with Monte Carlo data for $V^{\text{eff cl}}(x_0)$ [13]. Except for very low temperatures $T \lesssim 1/20$, the agreement is excellent. Note the significant improvement in going from $W_1(x_0)$ to $W_3(x_0)$.

To study the level splitting due to tunneling we go to the zero-temperature limit where the approximation is expected to be the worst. In this limit, $W_3(x_0)$ reduces to

$$\begin{aligned}
W_3 &= V + \frac{\hbar\Omega}{2} + \frac{g_2}{2}a^2 + \frac{g_4}{8}a^4 \\
& - \frac{1}{2\hbar\Omega} \left[\frac{g_2^2}{2}a^4 + \frac{g_2g_4}{2}a^6 + \frac{g_3^2}{6}\frac{2}{3}a^4 + \frac{g_4^2}{24}\frac{1}{2}a^8 \right] \\
& + \frac{1}{6\hbar\Omega^2} \left[g_2^3\frac{3}{2}a^6 + g_2g_3^2\frac{4}{3}a^8 + g_2^2g_43a^8 + g_3^2g_4\frac{13}{3}a^{10} + g_2g_4^2\frac{35}{16}a^{10} + g_4^3\frac{37}{64}a^{12} \right]
\end{aligned} \tag{5}$$

with $a^2 = \hbar/2\Omega$. The arguments x_0 have been omitted, for brevity.

For the double-well

$$g_2 = \omega^2 - \Omega^2(x_0) + 3gx_0^2, \quad g_3 = 6gx_0, \quad g_4 = 6g. \tag{6}$$

For $g > g_c \approx 0.3$, the energy has a minimum at $x_0 = 0$. For $g \leq g_c$, there is an additional symmetric pair of minima at $x_0 = \pm x_m \neq 0$ [see Figs. 5.5

and 5.6 of Ref. [2] or [5]). The optimal Ω value, called Ω_3 , is found by setting $\partial W_3/\partial\Omega = 0$ at each minimum. The resulting $W_3(0)$ is plotted in Fig. 2a together with $W_1(0)$ obtained from the original Feynman-Kleinert approximation, which contains only the first line of (5). More explicitly, this energy is (in natural units $\hbar = 1, \omega^2 = -1$)

$$W_1(0) = \frac{\Omega}{4} - \frac{1}{4\Omega} + \frac{3g}{4}a^4. \quad (7)$$

with $a^2 = 1/2\Omega$. The optimal Ω satisfies $\Omega^2 = -1 + 3ga^2$.

We also plot the first excited energy obtained from a corresponding variational treatment of the perturbatively calculated energy (see Ref. [5]).

At small g , the energies $W_1(0)$, $W_3(0)$, ... diverge and the minima at the nonzero values $x = \pm x_m$ become relevant. Moreover, there is quantum tunneling across the central barrier from one minimum to the other. This occurs for $g \leq g_c \approx 0.34$ and is unaccounted for by $W_3(0)$ and $W_3(x_m)$. Tunneling leads to a level splitting which in the classical limit is given by

$$\Delta_0 E(\omega) = 48 \sqrt{\frac{\omega_m^2/3g\hbar}{2\pi}} \hbar \omega_m e^{-\omega_m^2/3g\hbar} \quad (8)$$

where $\omega_m^2 = -2\omega^2$ is the curvature at the classical minimum [15]. The first loop correction improves this to

$$\Delta_1 E(\omega) = 48 \sqrt{\frac{\omega_m^2/3g\hbar}{2\pi}} \hbar \omega_m e^{-\omega_m^2/3g\hbar - (71/24)g\hbar/\omega_m^2} \quad (9)$$

In Fig. 2b we have plotted the energies

$$E_1^{0,1} = W_1(x_m) \pm \Delta_0 E(\omega_m)/2 \quad (10)$$

and

$$E_3^{0,1} = W_3(x_m) \pm \Delta_1 E(\omega_m)/2 \quad (11)$$

and see that while $\Delta_0 E(\omega_m)$ grossly overestimates the level splitting for $g \approx 0.3$, the splitting $\Delta_1 E(\omega_m)/2$ leads to reasonable energies $E_3^{0,1}$.

For completeness we have also tried to incorporate the level splitting formula into the variational treatment by rewriting $\Delta_1 E$ with the trivial substitution

$$\omega_m^2 = \Omega^2 - 2\omega^2 - \Omega^2 \equiv \Omega^2 + gr \quad (12)$$

as

$$\Delta_1 E(\Omega) = 48 \sqrt{\frac{\Omega^3/3g\hbar}{2\pi}} \hbar \Omega e^{-(\Omega^2+gr)^{3/2}/3g\hbar + \frac{1}{2} \log(gr\hbar/\Omega^3) - (71/24)gr/(\Omega^2+gr)^{1/2}} \quad (13)$$

and expanding the exponent in powers of g up to the first order. The energies of the two lowest states are then

$$E_{3v}^{0,1} = W_3(x_m) \pm \Delta_1 E(\Omega_3)/2. \quad (14)$$

with $x_m, \Omega(x_m)$ minimizing $W_3(x_0)$. The curves are shown in Fig. 2b.

For comparison we also display approximations based on $W_1(x_m)$. The lowest one is very easy to calculate. The first line of (5) reads explicitly

$$W_1(x_0) = \frac{x_0^2}{2} + \frac{a}{4}x_0^4 + \frac{\Omega}{2} + \frac{1}{2}(\omega^2 - \Omega^2 + 3gx_0^2)a^2 + 3\frac{g}{4}a^4 \quad (15)$$

The symmetric pair of minima in x_0 lies at

$$x_0 = \pm x_m = \pm \sqrt{(1 - 3ga^2)/g} \quad (16)$$

and has an energy

$$W_1(x_m) = -\frac{(1 - 3ga^2)}{4g} + \frac{\Omega}{4} - \frac{1}{4\Omega} + \frac{3g}{4}a^4. \quad (17)$$

The best Ω -value satisfies

$$\Omega = -1 + 3ax_m^2 + 3aa^2 = 2 - 6ga^2 \quad (18)$$

and has a real solution, to be called Ω_1 , for $g < g_c = (4/9)\sqrt{2/3} \approx 0.3629$. The curves are displayed in Fig. 2b, together with some lower approximations based on $W_1(x_m)$ explained in the figure caption. To see the effect of the expansion in the exponent of (13), we have introduced $\Delta'_1 E(\Omega)$, in which the exponent of (13) is expanded only up to the zeroth order in g . Fig 2b shows that this splitting is still too large.

Note that $W_1(x_m)$ does not possess the correct lowest-order behavior in g (failing to reproduce the slope by 25%) as can be seen in Fig. 2b. In fact, a Taylor expansion of $W_1(x_m)$ reads:

$$W_1(x_m) = \frac{\sqrt{2}}{2} - \frac{3}{16}g - \frac{9\sqrt{2}}{128}g^2 - \frac{27}{256}g^3 + \dots$$

with $\Omega(x_m) = \sqrt{2} - \frac{3}{4}g - \frac{2\sqrt{2}}{64}g^2 - \frac{27}{32}g^3 + \dots$. The deviation is due to the fact that coupling g_2 in Eq. (6) is of the order $\sqrt{g}$ so that its inclusion to second order is needed to obtain the correct slope.

A combined minimization of (14) yields, incidentally, worse results than those given here.

More details will be published in the forthcoming second edition of the textbook [2].

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Figure 2: Comparison of the variational energies of lowest two double-well states with numeric solutions of the Schrödinger equation indicated by fat dots. For $a > 0.3$, the central barrier is so low that no tunneling is required to cross. In Part a) of the figure shows the two limit cases $W_1(0)$ (dashed) and $W_3(0)$ (solid). Part b) of the figure magnifies the tunneling regime. The dotted curves represent $W_3(x_m) \pm \Delta_1 E(\omega_m)/2$. The solid curves arise from $W_3(x_m)$ by adding $\pm \Delta_1 E(\Omega_3)/2$ of Eq. (13) with the exponent expanded up to first order in g and Ω_3 and x_m minimizing $W_3(x_0)$. The broken curves represent lower approximations based on $W_1(x_m)$ —Curve 1: with an added semiclassical $\pm \Delta_0 E(\omega_m)/2$, Curve 2 with an added $\pm \Delta_0 E(\Omega_1)/2$, Curve 3 with $\pm \Delta_1' E(\Omega_1)/2$, and Curve 4 with $\pm \Delta_1 E(\Omega_1)/2$, respectively [Ω_1 and x_m optimize $W_1(x_m)$]. Note that the curves 1–4 based on $W_1(x_m)$ fail to reproduce the initial slope by 25%. The two central curves represent $W_1(x_m)$ (dashed) and $W_3(x_m)$ (dash-dotted) without level splitting.

Figure 1: Comparison of approximate effective classical potential $W_1(x_0)$ (dashed) and $W_3(x_0)$ (solid) at various inverse temperatures $\beta = 1/T$ with the exact one (dots) obtained numerically via Monte Carlo simulations based on averages over 10^5 configurations. The data points are from [12]. We have picked the worst case $g = 0.4$.