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Comment

Comment on 'Improving series convergence: the simple pendulum and beyond'

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Abstract

In this comment we analyze the improved series proposed by Duki *et al* (2018 *Eur. J. Phys.* **39** 065802) for the approximate calculation of a variety of physical quantities like the period of the simple pendulum and an integral of the exponential of a two-dimensional potential-energy function. We show that the application of the approach to the latter case is unnecessary because both the expansion coefficients and the original problem are given in terms of a similar error function. Present results for the straightforward expansion with exact analytic coefficients do not show the oscillatory behaviour exhibited by the calculations of those authors. We give reasons why the improved approach of Duki *et al* may not be suitable for the treatment of many realistic physical problems.

Keywords: perturbation theory, improved series, expansion point

1. Introduction

In a recent paper, Duki *et al* [1] proposed a simple method for improving the rate of convergence of power series that are commonly used to solve some problems in physics. The approach consists of expanding the physical quantity about a more convenient point. The authors applied the technique to the period of the simple pendulum and to an integral of the exponential of the potential known as Mexican hat. They claimed that their 'improved series' converges more rapidly than the 'regular' one.

The improved series applied to the simple pendulum is quite similar to a more general one proposed several years ago in this same journal [2]. However, this comment focuses on the

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second problem just mentioned. In section 2 we discuss this example and in section 3 we summarize the main results and draw conclusions.

2. Example

The example we want to discuss here is the integral

$$\Delta = 2\pi \int_0^\infty e^{-\beta U(r)} r \mathrm{d}r, \tag{1}$$

where $U(r) = -ar^2 + br^4$ and $r = \sqrt{x^2 + y^2}$. In terms of the variable $\xi = r^2$ this integral becomes

$$\Delta = \pi \int_0^\infty e^{\beta a\xi - \beta b\xi^2} \mathrm{d}\xi. \tag{2}$$

If we expand $e^{\beta a\xi}$ in a Taylor series about $\xi = 0$ we obtain what the authors call the 'regular' expansion

$$\Delta = \pi \sum_{j=0}^{\infty} \frac{(\beta a)^j}{j!} \int_0^\infty \xi^j e^{-\beta b\xi^2} \mathrm{d}\xi. \tag{3}$$

Note that all the coefficients of this convergent expansion can be calculated exactly (see below).

The authors decided to improve the rate of convergence of the series by expanding about an alternative point. To this end they rewrote the integral in terms of the variable $\xi - \xi_0$ for $a = 1/2$ and $b = 1/4$. A straightforward calculation shows that

$$\Delta = \pi e^{\frac{\beta}{4}\xi_0(2-\xi_0)} \int_0^\infty e^{\frac{\beta}{2}(1-\xi_0)(\xi-\xi_0) - \frac{\beta}{4}(\xi-\xi_0)^2} \mathrm{d}\xi. \tag{4}$$

Note that two factors in this equation slightly differ from the corresponding ones derived by Duki *et al* [1]; however, this difference is irrelevant for present discussion. If we expand $e^{\frac{\beta}{2}(1-\xi_0)(\xi-\xi_0)}$ in a Taylor series about $\xi = \xi_0$ we obtain an improved expansion with coefficients that are proportional to the integrals

$$I_n = \int_0^\infty (\xi - \xi_0)^n e^{-\frac{\beta}{4}(\xi-\xi_0)^2} \mathrm{d}\xi, \quad n = 0, 1, \ldots \tag{5}$$

The authors claimed that this expansion converges more rapidly than the regular one but they forgot to mention an important difference between both approaches. The coefficients of even order of the improved expansion cannot be calculated in exact analytical way because they depend on the error function $\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} \mathrm{d}t$; for example:

$$\begin{aligned} I_0 &= \frac{\sqrt{\pi}}{\sqrt{\beta}} \left[1 + \mathrm{erf}\left(\frac{\sqrt{\beta}\xi_0}{2}\right)\right] \\ I_1 &= \frac{2e^{\frac{-\beta\xi_0^2}{4}}}{\beta} \\ I_2 &= \frac{2\sqrt{\pi}}{\beta^{\frac{3}{2}}} \left[1 + \mathrm{erf}\left(\frac{\sqrt{\beta}\xi_0}{2}\right)\right] - \frac{2\xi_0}{\beta} e^{\frac{-\beta\xi_0^2}{4}}. \end{aligned} \tag{6}$$

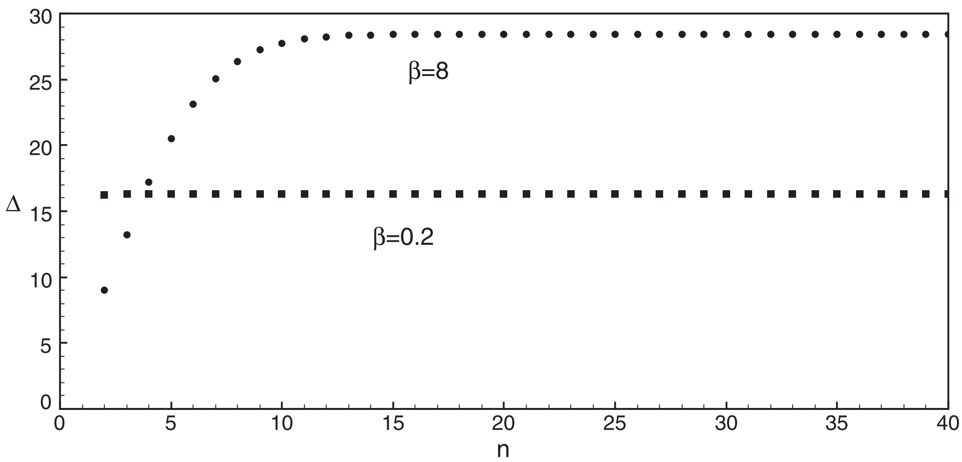

Figure 1. Partial sums of order n for the regular series with $a = 1/2$, $b = 1/4$ and two values of β.

The original problem consists of an integral Δ that should be calculated numerically (more details below) and Duki *et al* proposed to approach it by an expansion where half of the coefficients are given by integrals that should be calculated numerically. One may conclude that the improved approach does not represent a great advantage in this case.

The regular approach can be rewritten in a more convenient way. If we define the new integration variable $x = \sqrt{\beta b} r^2$, then we obtain the more compact expression

$$\Delta(a, b, \beta) = \frac{\pi}{\sqrt{\beta b}} I(\lambda), \ \lambda = a\sqrt{\frac{\beta}{b}}$$
$$I(\lambda) = \int_0^\infty e^{\lambda x} e^{-x^2} dx. \tag{7}$$

We appreciate that the essential part of Δ is an integral that depends on just one variable that combines the three parameters of the problem. This fact considerably simplifies the analysis and comparison of the different approaches that we can apply to the problem. In particular note that

$$I(\lambda) = \frac{\sqrt{\pi}}{2} e^{\frac{\lambda^2}{4}} \left[\text{erf}\left(\frac{\lambda}{2}\right) + 1 \right]. \tag{8}$$

Clearly, the calculation of Δ requires the calculation of an error function. Since the improved approach proposed by Duki *et al* [1] also requires the calculation of an error function it does not seem to be worth the effort.

The regular approach can now be written in compact form as

$$\Delta(a, b, \beta) = \frac{\pi}{2\sqrt{\beta b}} \sum_{n=0}^{\infty} \Gamma\left(\frac{n+1}{2}\right) \lambda^n, \tag{9}$$

where all the coefficients have an exact analytical expression as indicated above.

Since all the terms in the regular expansion are positive one does not expect the partial sums to oscillate as shown in figure 4 of Duki *et al* [1]. In figure 1 we show the actual behaviour of the partial sums for $\beta = 0.2$ and $\beta = 8$ (in both cases $a = 1/2$ and $b = 1/4$ as chosen by Duki *et al*). Present results differ considerably from the ones of those authors.

3. Conclusions

In this comment we wanted to prove the following facts. First, that the improved series proposed by Duki *et al* does not represent an advantage in the case of the calculation of the integral Δ. The reason is that the coefficients of the improved series are given in terms of an error function that is similar to the one required to obtain the exact result. Second, that their calculation of the regular series exhibits an oscillatory behaviour that is inconsistent with the fact that all the terms of this series are positive.

Finally, we want to show that a mere shift of the expansion variable is not practical in many realistic problems. For example, in the application of perturbation theory to some quantum-mechanical models we write the Hamiltonian operator in the form $H(\lambda) = H_0 + \lambda H'$ and expand the eigenvalues and eigenfunctions of the corresponding Schrödinger equation in a Taylor series about $\lambda = 0$. This approach is particularly useful when we can solve the Schrödinger equation for $H(0) = H_0$ exactly [3]. If we want to expand the solutions about a different point $\lambda = \lambda_0$ then we need the eigenvalues and eigenfunctions of the Hamiltonian operator $H(\lambda_0)$. But this is precisely the problem that we cannot solve exactly. This example matches the situation described above about the much simpler integral Δ.

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