He’s amazing calculations with the Ritz method

Paolo Amore∗

Facultad de Ciencias, Universidad de Colima, Bernal Díaz del Castillo 340, Colima, Colima, Mexico

Francisco M. Fernández†

INIFTA (UNLP, CCT La Plata-CONICET), División Química Teórica, Diag. 113 y 64 (S/N), Sucursal 4, Casilla de Correo 16, 1900 La Plata, Argentina

We discuss an earlier application of the Ritz variational method for strongly nonlinear problems. We clearly prove that the results derived for several extremely simple problems of supposedly physical and mathematical interest do not provide any clue on the utility of the approach.

1. Introduction

In a recent review in this journal, He [1] analyzed several asymptotic methods for strongly nonlinear equations. One such approach, the so called Ritz method, consists mainly in converting the nonlinear differential equation into a Newton equation of motion. Thus, by minimization of the action integral for the Lagrangian function one obtains an approximate solution to the nonlinear equation that is expected to be optimal from a variational point of view. Obviously, the accuracy of the approximate solution depends heavily on the chosen variational ansatz or trial “trajectory”.

The purpose of this paper is to analyze the Ritz method proposed by He [1] and determine if it is already useful for solving actual nonlinear problems. For the sake

∗paolo.amore@gmail.com
†fernande@quimica.unlp.edu.ar
of clarity in what follows we devote a section to each of the problems discussed.

2. Anharmonic oscillator

First, He [1] transforms the equation of motion for the Duffing oscillator

\[ \ddot{u}(t) - u(t) + \epsilon u(t)^3 = 0 \quad (1) \]

into the variational integral

\[ J(u) = \int \left( -\frac{1}{2} \dot{u}^2 - \frac{1}{2} u^2 + \frac{\epsilon}{4} u^4 \right) dt \quad (2) \]

and concludes that “it requires that the potential \( V(u) = -u^2/2 + \epsilon u^4/4 \) must be positive for all \( t > 0 \), so an oscillation about the origin will occur only if \( \epsilon A^2 > 2 \), where \( A \) is the amplitude of the oscillation”. Unfortunately, He [1] does not show the trial function from which he draws that conclusion.

The Duffing oscillator has been widely studied and, consequently, its properties are well known [2]. For example, from straightforward inspection of the potential \( V(u) \) we already know that there is an unstable equilibrium point at \( u = 0 \) when \( \epsilon < 0 \). On the other hand, when \( \epsilon > 0 \) the potential \( V(u) \) exhibits a local maximum \( V = 0 \) at \( u = 0 \) and two minima of depth \( -1/(4\epsilon) \) symmetrically located at \( \pm 1/\sqrt{\epsilon} \).

If the initial conditions are such that \( V(A) > 0 \) then the oscillation will certainly be about the origin; otherwise there will be oscillations about one of the two minima. It is clear that by simple inspection of the potential we obtain much more information that the one derived by He [1] from the action integral. Therefore, He’s application of the Ritz method to this model is of no relevance whatsoever.

3. A chemical reaction

He [1] proposed the application of the Ritz method to the chemical reaction

\[ nA \rightarrow C + D \quad (3) \]

If \( N_A(t), N_B(t), \) and \( N_C(t) \) are the number of molecules of the species \( A, B, \) and \( C \), respectively, at time \( t \) then He [1] assumed that \( N_A(0) = a, \) and \( N_B(0) = N_C(0) = 0. \)
If we call \( x = N_B(t) = N_C(t) \), then we conclude that \( N_A(t) = a - nx \), where \( x \) is known as the extent of reaction [3, 4]. The unique rate of reaction can be defined in terms of the extent of reaction as \( v = dx/dt \). He [1] further assumed that the rate law is given by

\[
\frac{dx}{dt} = k(a - x)^n
\]  

(4)

At this point we stress the fact that this expression is correct only if the chemical reaction (3) is elementary, otherwise the rate law may be more complicated. Most chemical reactions are not elementary and therefore the reaction order and molecularity do not necessarily agree, as discussed in any book on physical chemistry [3] or chemical kinetics [4]. What is more, the order of reaction may not even be a positive integer [3, 4]. For concreteness here we assume that the rate law (4) is correct.

He [1] obtained an approximate solution to the differential equation (4) by means of the action integral

\[
J = \frac{1}{2} \int_0^\infty \left[ \left( \frac{dx}{dt} \right)^2 + k^2(a - x)^{2n} \right] dt
\]  

(5)

and the variational ansatz

\[
x_{\text{var}} = a \left( 1 - e^{-\eta t} \right)
\]  

(6)

where \( \eta \) is a variational parameter. Notice that \( x_{\text{var}}(t) \) satisfies the boundary conditions at \( t = 0 \) and \( t \to \infty \). He [1] found that the optimal value of the effective first–order rate constant \( \eta \) was given by

\[
\eta = \frac{ka^{n-1}}{\sqrt{n}}
\]  

(7)

Furthermore, He [1] argued that chemists and technologists always want to know the half–time \( t_{1/2} = t(x = a/2) \) (which he called halfway time). According to equations (6) and (7) the half–time is given approximately by

\[
t_{1/2} = \frac{\sqrt{n \ln(1/2)}}{k a^{n-1}}
\]  

(8)

According to He [1] the exact reaction extent for \( n = 2 \) is

\[
x_{He}^{\text{exact}}(n = 2) = a \left( 1 - \frac{1}{1 - k a t} \right)
\]  

(9)
This result is obviously wrong because it exhibits an unphysical pole at \( t = 1/(ka) \).

From this incorrect expression He [1] derived a meaningless negative half–time

\[ t_{1/2}^{He}(n = 2) = -\frac{1}{ka} \]  

(10)

In order to obtain a reasonable agreement with the variational result (8) He [1] then carried out the following wrong calculation

\[ t_{1/2}^{var}(n = 2) = -\frac{\sqrt{2}\ln(1/2)}{ka^{n-1}} = -\frac{0.98}{ka} \]  

(11)

In this way He [1] managed to obtain two unphysical negative half–times that agreed 98%.

Disregarding the mistakes outlined above we may ask ourselves whether the approximate variational result may be of any utility to a chemist. Any textbook on physical chemistry [3] or chemical kinetics [4] shows that the exact solution to equation (4) is

\[ x_{exact} = a \left\{1 - \frac{1}{1 + k(n-1)a^{n-1}t^{1/(n-1)}}\right\}, n \neq 1 \]  

(12)

and that the exact half–time is given by

\[ t_{1/2}^{exact} = \frac{2^{n-1} - 1}{k(n-1)a^{n-1}} \]  

(13)

It is common practice in chemistry to estimate the half–time from experimental data in order to determine the order of the reaction. Obviously, an inaccurate expression would lead to an inexact order of reaction.

The variational half–time (8) is reasonably accurate for \( n = 2 \) because it is exact for \( n = 1 \). The reason is that the variational ansatz (6) is the exact solution for a first–order reaction when \( \eta = k \). Notice that equation (7) leads to such a result when \( n = 1 \). We can easily verify that the ratio \( t_{1/2}^{var}/t_{1/2}^{exact} \) increasingly deviates from unity as \( n \) increases. Therefore, \( n = 2 \) (the only case selected by He [4]) is the most favorable case if \( n \) is restricted to positive integers greater than unity.

The half–time (or half–life) is a particular case of partial reaction times. We may, for example, calculate the time \( t = t_{1/4} \) that has to elapse for the number of
A molecules to reduce to $a/4$ ($x = 3a/4$). It is not difficult to verify that

$$\frac{t_{\text{exact}}^{1/4}}{t_{\text{exact}}^{1/2}} = 2^{n-1} + 1 \quad (14)$$

From the experimental measure of $t_{1/2}$ and $t_{1/4}$ chemists are able to obtain the reaction order $n$. However, if they used He’s variational expression (6) they would obtain

$$\frac{t_{\text{var}}^{1/4}}{t_{\text{var}}^{1/2}} = 2 \quad (15)$$

that is useless for $n \neq 1$. According to what we have said above it is not surprising that this ratio is exact for $n = 1$. We clearly appreciate that the variational result does not provide the kind of information that chemists would like to have because it only predicts first-order reactions.

From the discussion above we conclude that no chemist will resort to the variational expressions in the study of chemical reactions. There is no reason whatsoever for the use of an unreliable approximate expression when one has a simple exact analytical one at hand. Besides, we have clearly proved that the variational expressions are utterly misleading.

4. Lambert equation

He [1] also applied the Ritz method to the Lambert equation

$$y''(x) + \frac{k^2}{n}y(x) = (1 - n)\frac{y'(x)^2}{y(x)} \quad (16)$$

and arrived at the variational formulation

$$J(y) = \frac{1}{2} \int (-n^2y^{2n-2}y'^2 + k^2y^{2n}) \, dt \quad (17)$$

By means of the transformation $z = y^n$ He obtained

$$J(z) = \frac{1}{2} \int (-z'^2 + k^2z^2) \, dt \quad (18)$$

that leads to the Euler–Lagrange equation

$$z'' + k^2z = 0 \quad (19)$$
Obviously, the solution to this linear equation is straightforward.

If we substitute the transformation $z = y^n$ into equation (16) we obtain equation (19) in a more direct way. Therefore, there is no necessity for the variational Ritz method.

5. Soliton solution

He [1] also studied the KdV equation

$$\frac{\partial u(x,t)}{\partial t} - 6u(x,t)\frac{\partial u(x,t)}{\partial x} + \frac{\partial^3 u(x,t)}{\partial x^3} = 0$$

(20)

and looked for its travelling–wave solutions in the frame

$$u(x,t) = u(\xi), \xi = x - ct$$

(21)

The function $u(\xi)$ satisfies the nonlinear ordinary differential equation

$$u'''(\xi) - cu'(\xi) - 6u(\xi)u'(\xi) = 0$$

(22)

where the prime indicates differentiation with respect to $\xi$. Then He [1] integrated this equation (taking the integration constant arbitrarily equal to zero) and obtained

$$u''(\xi) - cu(\xi) - 3u(\xi)^2 = 0$$

(23)

By means of the so called semi–inverse method He [1] obtained the variational integral

$$J = \int_0^{\infty} \left[ \frac{1}{2} \left( \frac{du}{d\xi} \right)^2 + \frac{c}{2} u^2 + u^3 \right] dt$$

(24)

Choosing the trial function

$$u = p \cosh^{-2}(q\xi)$$

(25)

where $p$ and $q$ are variational parameters, He [1] obtained $p = c/2$ and $q = \sqrt{c}/2$.

By substitution of equation (25) into equation (22) we obtain the same values of $p$ and $q$ in a more direct way and with less effort. Therefore, there is no need for the variational method for the successful treatment of this problem.
6. Bifurcation

He [1] also applied the Ritz method to the most popular Bratu equation

\[ u''(x) + \lambda e^{u(x)} = 0, \quad u(0) = u(1) = 0 \]  \hspace{1cm} (26)

that has been studied by several authors [5] (and references therein). Here we only cite those papers that are relevant to present discussion. He [1] derived the action integral

\[ J = \int_0^1 \left( \frac{1}{2} u'^2 - \lambda e^u \right) \, dx \]  \hspace{1cm} (27)

and proposed the simplest trial function that satisfies the boundary conditions:

\[ u(x) = Ax(1 - x) \]  \hspace{1cm} (28)

Curiously, He [1] appeared to be unable to obtain an exact analytical solution for the integral; however, it is not difficult to show that

\[ J(A) = \frac{A^2}{6} - \frac{\pi^{1/2} \lambda e^{A^4/4} \text{erf}(\sqrt{\pi}/2)}{A} \]  \hspace{1cm} (29)

We cannot exactly solve \( dJ(A)/dA = 0 \) for \( A \) but we can solve it for \( \lambda \):

\[ \lambda = \frac{4A^{5/2}}{3 \left[ \sqrt{\pi} (A - 2)e^{A^4/4} \text{erf}(\sqrt{\pi}/2) + 2\sqrt{A} \right]} \]  \hspace{1cm} (30)

The analysis of this expression shows that \( \lambda(A) \) exhibits a maximum \( \lambda_c = 3.569086042 \) at \( A_c = 4.727715383 \). Therefore there are two variational solutions for each \( 0 < \lambda < \lambda_c \), only one for \( \lambda = \lambda_c \) and none for \( \lambda > \lambda_c \). This conclusion agrees with the rigorous mathematical analysis of the exact solution [5] that we will discuss below. Besides, the critical value of the adjustable parameter \( A_c \) is also a root of \( d^2J(A)/dA^2 = 0 \).

The exact solution to the one-dimensional Bratu equation [26] is well-known. Curiously enough, He [1], Deeba et al [6], and Khury [7] showed a wrong expression. A correct one is (notice that one can write it in different ways)

\[ u(x) = -2 \ln \left\{ \frac{\cosh(\theta(x - 1/2))}{\cosh(\theta/2)} \right\} \]  \hspace{1cm} (31)
where $\theta$ is a solution to

$$\lambda = \frac{2\theta^2}{\cosh(\theta/2)^2}$$

(32)

The critical $\lambda$-value is the maximum of $\lambda(\theta)$, and we easily obtain it from the root of $d\lambda(\theta)/d\theta = 0$ that is given by

$$e^{\theta_c} (\theta_c - 2) - \theta_c - 2 = 0$$

(33)

The exact critical parameters are $\theta_c = 2.399357280$ and $\lambda_c = 3.513830719$ that lead to $u'(0)_c = 4$. We appreciate that the variational approach provides a reasonable qualitative (or even semi quantitative) description of the problem.

We may try a perturbation approach to the Bratu equation in the form of a Taylor series in the parameter $\lambda$:

$$u(x) = \sum_{j=0}^{\infty} u_j(x) \lambda^j$$

(34)

where, obviously, $u_0(x) = 0$. From the exact expression we obtain

$$u'(0) = \frac{\lambda}{2} + \frac{\lambda^2}{24} + \frac{\lambda^3}{160} + \ldots \approx 0.5\lambda + 0.0417\lambda^2 + 0.00625\lambda^3 + \ldots$$

(35)

while the variational approach also yields a reasonable result

$$u'(0) = \frac{\lambda}{2} + \frac{\lambda^2}{20} + \frac{43\lambda^3}{5600} + \ldots \approx 0.5\lambda + 0.05\lambda^2 + 0.00768\lambda^3 + \ldots$$

(36)

It seems that the Ritz method already produces satisfactory results for this kind of two-point boundary value problems.

Another simple variational function that satisfies the same boundary conditions is

$$u(x) = A \sin(\pi x)$$

(37)

It leads to the following variational integral:

$$J(A) = \frac{A^2 \pi^2}{4} - \lambda [I_0(A) + L_0(A)]$$

(38)

where $I_\nu(z)$ and $L_\nu(z)$ stand for the modified Bessel and Struve functions $[8]$, respectively. From the minimum condition we obtain

$$\lambda = \frac{A\pi^3}{2 \{2 + \pi [I_1(A) + L_1(A)]\}}$$

(39)
It is not difficult to show that this trial function yields better critical parameters: 
\[ \lambda_c = 3.509329130 \] and \[ u'(0)_c = 3.756549365. \] Besides, one can easily derive the approximate perturbation expansion exactly

\[
u'(0) = \frac{4\lambda}{\pi^2} + \frac{4\lambda^2}{\pi^4} + \frac{4\left(3\pi^2 + 16\right)\lambda^3}{3\pi^8} + \frac{4\left(\pi^2 + 18\right)\lambda^4}{\pi^{10}} + \ldots
\]

\[ \approx 0.405\lambda + 0.0411\lambda^2 + 0.00641\lambda^3 + \ldots \] (40)

Notice that although the coefficient of \( \lambda \) is not exact the remaining ones are more accurate than those of the preceding trial function.

Fig. 1 shows the exact slope at origin \( u'(0) \) in terms of \( \lambda \) and the corresponding estimates given by the two variational functions. We appreciate that the variational approach proposed by He [1] yields the solution with smaller \( u'(0) \) (lower branch) more accurately than the other one (upper branch). This comparison between the exact and approximate solutions for a wide range of values of \( \lambda \) was not carried out before; He [1] simply compared the two slopes at origin for just \( \lambda = 1 \). The other trial function (37) yields a better overall approximation at the expense of the accuracy for small values of \( \lambda \). Some more elaborated approaches, like the Adomian decomposition method, fail to provide the upper branch [6]; therefore, the Ritz method seems to be suitable for the analysis of this kind of nonlinear problems.

We may conclude that the Ritz variational method provides a useful insight into the Bratu equation. However, one should not forget that there is a relatively simple exact solution to this problem and that the generalization of the approach in the form of a power series proposed by He [1]

\[ u(x) = Ax(1-x)(1 + c_1x + c_2x^2 + \ldots) \] (41)

may surely lead to rather analytically intractable equations.

7. Conclusions

Historically, scientists have developed perturbational, variational and numerical approaches to solve nontrivial mathematical problems in applied mathematics and
theoretical physics. In some cases, where the exact solution exists but is given by complicated special functions, an approximate simpler analytical solution may nonetheless be of practical utility. However, He [1] chose examples where either the Ritz method does not provide any useful insight, or the exact analytical solutions are as simple as the approximate ones, or the direct derivation of the exact result is more straightforward than the use of the variational method. From the discussions in the preceding sections we may conclude that He’s application of the Ritz variational method [4] does not show that the approach is suitable for the treatment of nonlinear problems. In most of the cases studied here the straightforward analysis of the problem yields either more information or the same result in a more direct way.

To be fair we should mention that the Ritz variational method provides a reasonable bifurcation diagram by means of relatively simple trial functions as shown in Fig. [1]. However, even in this case the utility of the approach is doubtful because there exists a remarkably simple analytical solution to that equation. The treatment of a nontrivial example is necessary to assert the validity of the approach.

He’s choice of the rate equation for chemical reactions [1] is by no means a happy one (without mentioning the mistakes in the calculations). In this case the exact solution is quite simple and the variational ansatz is unsuitable for practical applications. We may argue that a trial function with the correct asymptotic behaviour would yield meaningful results. In fact, it may even produce the exact result; but one should not forget that such a success would obviously be due to the fact that there exist a remarkably simple exact solution available by straightforward integration.

As said before, present results show that He [1] failed to prove that the Ritz variational method provides a successful way of treating strongly nonlinear problems. Of course, the main ideas behind that variational method are correct, and the case of Bratu equation suggests that it may be possible to find appropriate trial functions for the successful treatment of some problems. Unfortunately, the remaining
He’s choices [1] do not do much to convince one that the method is worthwhile.

He’s article [1] is an example of the kind of poor research papers that have been lately published by some supposedly respectable journals. It is part of such journals’ policy to reject comments that can reveal this unfortunate situation. One may ask oneself what is the profit that those journals get from such a practice. If the reader is interested in other examples of poor research papers in supposedly respectable journals I suggest some earlier reports in this forum [9–14].

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Fig. 1. Bifurcation diagram for the slope at origin $u'(0)$ in terms of $\lambda$