Comment on: “Development of the perturbation theory using polynomial solutions”

[J. Math. Phys. 60, 012103 (2019)]

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The purpose of this comment is to present the perturbation approach proposed by Maiz [J. Math. Phys. 60, 012103 (2019)] in a clearer way. The results of our straightforward procedure agree with those obtained by that author except for one case in which we obtain the exact result while he obtained an approximate one. In addition to it, we show that for sufficiently deep double-well potentials the perturbation approach deteriorates considerably.

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I. INTRODUCTION

In a recent paper Maiz proposed a modified perturbation approach in which the unperturbed or reference Hamiltonian operator is chosen to be somewhat close to the actual, or perturbed, Hamiltonian operator. The method, named exact polynomial potential solutions (EPPS from now on), was restricted to one-dimensional polynomial potentials. Numerical results of first order in perturbation theory appear to be reasonably accurate for a family of anharmonic oscillators.

In our opinion the author presents the approach in a somewhat unclear and confusing way. The purpose of this comment is to develop that perturbation strategy more clearly. In section II we present the method and apply it to the set of anharmonic oscillators discussed in that paper. In section III we summarize the main conclusions and show results for some examples not considered by Maiz.

II. EXACT POLYNOMIAL POTENTIAL SOLUTIONS

In what follows we just focus on the dimensionless Schrödinger equation

\[ \psi''(x) = [V(x) - E] \psi(x), \]
\[ V(x) = \sum_{i=1}^{N} b_i x^i, \] (1)

where \( N \) is an even number and \( b_N > 0 \). Maiz proposed an ansatz of the form

\[ \psi(x) = f(x) \exp[h(x)], \]
\[ h(x) = \sum_{i=1}^{2N} a_i x^i, \] (2)

where \( f(x) = 1 \) for the ground state and \( f(x) = \prod_{i=1}^{n} (x - x_i) \) for the excited states. In this way the author derived a quasi-exactly-solvable Hamiltonian \( H_{ex} \) and then improved the exactly known eigenvalue \( E^{(0)} \) of \( H_{ex} \) by means of
perturbation theory of first order: \( E^{(1)} = \langle H - E_{\text{ex}} \rangle \). It is clear that one needs a recipe for the calculation of optimal values of the parameters in the ansatz. As stated in the introduction we think that the author’s presentation of his method is rather unclear and the purpose of this comment is to develop it in a somewhat clearer way.

The starting point is a square-integrable trial function \( \varphi(x, a) \) where \( a \) is a set of adjustable parameters. From this function we derive a potential \( V_0(x, a) \) as

\[
\frac{\varphi''(x, a)}{\varphi(x, a)} = V_0(x, a) - E^{(0)}(a). \tag{3}
\]

Then we obtain a correction of first order in the usual way

\[
E^{(1)} = \frac{\int_{-\infty}^{\infty} [V(x) - V_0(x, a)] \varphi(x, a)^2 \, dx}{\int_{-\infty}^{\infty} \varphi(x, a)^2 \, dx}. \tag{4}
\]

The accuracy of the result will obviously depend on the choice of the adjustable parameters \( a \).

The equations developed above are quite general (in fact, once can easily write similar equations for more than one dynamical coordinate), but in what follows we restrict ourselves to the ground states of the polynomial potentials considered by Maiz. To this end we choose

\[
\varphi(x, a) = \exp\left[h(x, a)\right],
\]

\[
h(x, a) = \sum_{i=1}^{M} a_i x^i, \tag{5}
\]

where \( M \) is even and \( a_M > 0 \). The potential of order zero

\[
V_0(x, a) = h'(x, a)^2 - h''(x, a) + E^{(0)}(a), \tag{6}
\]

where \( E^{(0)}(a) = 2a_2 - a_1^2 \) and the prime stands for derivative with respect to \( x \), is a polynomial function of order \( 2M - 2 \). We arbitrarily choose the \( M \) adjustable parameters \( a = (a_1, a_2, \ldots, a_M) \) in order to remove \( M \) terms of the perturbation potential \( V(x) - V_0(x, a) \). In order to reproduce the results of Maiz we choose \( 2M - 2 > N \) and, obviously, \( a_{2j+1} = 0 \) if \( V(-x) = V(x) \).

Our first example is the exactly solvable harmonic oscillator \( V(x) = x^2 \). If \( M = 4 \) we have

\[
V(x) - V_0(x, a) = -16a_4^2 x^4 - 16a_2 a_4 x^2 - x^2 \left(4a_4^2 - 2a_2 - 1 \right), \tag{7}
\]

from which it follows that \( a_4 = 0 \) and \( a_2 = 1/2 \). We thus obtain, as expected, the exact ground state energy at zero order \( E^{(0)} = 1 \). Curiously enough, Maiz obtained an approximate result for this trivial case. At first sight it may seem that both approaches are different.

In the case of \( V(x) = x^4 \) we choose the same ansatz and obtain the following results

\[
a_2 = \frac{12^{1/3}}{4}, \quad a_4 = \frac{18^{1/3}}{24},
\]

\[
V(x) - V_0(x, a) = -\frac{12^{1/3}}{12} x^6 = -0.190785707x^6,
\]

\[
E_0 = \frac{12^{1/3}}{2} = 1.144714242, \tag{8}
\]

that exactly agree with those of Maiz. The calculation of \( E^{(1)} = -0.07198347757 \) should be carried out numerically and we appreciate that it also agrees with the result of that author. We thus have \( E = E^{(0)} + E^{(1)} = 1.072730764 \).
that closely agrees with accurate results obtained by other means (see also Table I to be discussed later on). Now it seems that our approach is identical to EPPS but we have not been able to find the source of the discrepancy in the case of the harmonic oscillator.

In the case of the potential $V(x) = x^2 + x^3 + x^4$ we also choose $M = 4$ but we include both even- and odd-parity terms. A straightforward numerical calculation shows that

$$a_1 = 0.22892176, \quad a_2 = 0.6805239186, \quad a_3 = 0.1038578221, \quad a_4 = 0.0829252897,$$

$$E_0 = 1.308642664, \quad V(x) - V_0(x,a) = -0.206698483x^5 - 0.1100255772x^6,$$  \hspace{1cm} (9)

in agreement with the results of EPPS, except for a slight discrepancy in the coefficient of $x^6$ that is probably due to numerical errors. We also obtain $E^{(1)} = 0.00471053228$ and $E = 1.313350717$ in perfect agreement with EPPS.

Present approach agrees with EPPS also in the case of the other models considered in that paper. In general, the results provided by this approach appear to be quite reasonable. In order to test the accuracy of his results Maiz resorted to reference eigenvalues obtained by means of other approach. However, in that paper there are results only for even-parity potentials. Table I shows accurate benchmark energies calculated by means of the Riccati-Padé method (RPM). We appreciate that Maiz’s reference eigenvalues are less accurate than the reported number of significant digits appears to suggest.

III. FURTHER COMMENTS AND CONCLUSIONS

It has been our purpose in this comment to develop the EPPS in a simpler and clearer way. In doing so we found out that Maiz should have obtained the exact result for the harmonic oscillator instead of the approximate one reported in his paper. The EPPS appears to yield reasonable results for the ground states of polynomial potentials by means of first-order perturbation theory. However, for such simple models one easily obtains very accurate results by means of the straightforward Raleigh-Ritz variational method or any other approach. Here we have resorted to the RPM that converges exponentially fast. The results in Table I were obtained from the roots of Hankel determinants of dimension $D \leq 10$.

In the case of double-well potentials the EPPS may perform poorly if the wells are sufficiently deep. For example, in the case of $V(x) = x^4 - \lambda x^2$ we obtain $(E^{[EPPS]} = 0.7122694296, E^{[RPM]} = 0.65765300518071512)$ for $\lambda = 1$ and $(E^{[EPPS]} = 0.885893999, E^{[RPM]} = 0.6389156378)$ for $\lambda = 5$. The percent errors 8.3 and 38.7, respectively, are considerably larger than those for the models chosen by Maiz.

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TABLE I: Reference ground-state eigenvalues calculated by means of two different approaches

| $V(x)$                      | Maiz$^2$    | RPM                       |
|-----------------------------|-------------|---------------------------|
| $x^4$                       | 1.06065     | 1.0603620904841829        |
| $x^2 + x^3 + x^4$           | 1.310342    | 1.31025752970575          |
| $x^6$                       | 1.14571     | 1.14480245380             |
| $x^2 + x^6$                 | 1.43555     | 1.43562461900             |
| $x^4 + x^5 + x^6$           | 1.3032      | 1.30272754246             |
| $x^2 - x^3 + x^4 + x^6$     | 1.586428    | 1.58657805318             |
| $x^2 - x^3 + x^4 - x^5 + x^6$ | 1.470961   | 1.4711571858              |