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Comment on "A new efficient method for calculating perturbative energies using functions which are not square integrable": regularization and justification

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Abstract

The method recently proposed by Skála and Čížek for calculating perturbation energies in a strict sense is ambiguous because it is expressed as a ratio of two quantities which are separately divergent. Even though this ratio comes out finite and gives the correct perturbation energies, the calculational process must be regularized to be justified. We examine one possible method of regularization and show that the proposed method gives traditional quantum mechanics results.

Recently, in a letter in this journal [1], Skála and Čížek (SC) proposed a method to calculate perturbation energies using non-sqaure-integrable functions. The method of SC is further augmented in a comment by Guardiola and Ros (GR) [2]. The purpose of our present comment is to further point out that in a strict sense, the SC method for the perturbation energies can result in a ratio of two divergent quantities, so that while this ratio may remain finite in a practical numerical calculation, a regularization procedure is needed to justify the finite result. We have examined one such possible regularization procedure and made contact between the SC method and traditional quantum mechanics (QM) results.

Briefly, the SC method regards the n-th order perturbation equation as a parametric differential equation with E_n as the parameter,

$$(H_0 - E_0)\psi_n(E_n, x) = (E_n - \tilde{V}_n)\psi_0(x), \tag{1}$$

where

$$H_0 = -\frac{d^2}{dx^2} + V_0, \tag{2}$$

and

$$\tilde{V}_n\psi_0 \equiv V_1\psi_{n-1} - \sum_{i=1}^{n-1} E_i\psi_{n-i}. \tag{3}$$

Here we have chosen to introduce $\tilde{V}_n$ as the effective perturbation in the n-th order equation. For $n = 1$, the sum in R.H.S. of Eq. (3) vanishes and $\tilde{V}_1$ is the same as the real perturbation V_1. We also adopt the convention that all the wavefunctions are physical unless the dependence on the parameter E_n is explicitly displayed. For this form of Eq. (1), the n-th order equation is similar in form to the first order equation. $\tilde{V}_n$ is a known function since all lower order quantities are assumed known. In traditional QM perturbation theory, one left multiplies Eq. (1) with the zeroth order wave function ψ_0. Under the usual normalization conditions,

$$\langle\psi_0|\psi_0\rangle = 1 \qquad \text{and} \qquad \langle\psi_0|\psi_i\rangle = 0 \quad \forall i \neq 0, \tag{4}$$

one recovers the standard QM result

$$E_n = \langle \psi_0 | \tilde{V}_n | \psi_0 \rangle = \langle \psi_0 | V_1 | \psi_{n-1} \rangle. \tag{5}$$

Once E_n is correctly obtained, $\psi_n(E_n, x)$ is obtained by solving the ordinary differential equation in Eq. (1).

SC propose that instead of obtaining E_n in the standard way first, one treats Eq. (1) as a parametric ordinary differential equation with E_n a parameter, and go on to show that

$$E_n = \frac{-\psi_n(0, x_0)}{\psi_n(1, x_0) - \psi_n(0, x_0)} \equiv \frac{-\psi_n(0, x_0)}{F(x_0)}, \tag{6}$$

where x_0 is a point such that the boundary conditions

$$\psi_n(E_n, x_0) = 0, \qquad n = 0, 1, \ldots \tag{7}$$

are met for the physicsal energies E_n. Since neither 0 nor 1 is the necessary n-th order energy correction E_n, the functions $\psi_n(0, x)$ and $\psi_n(1, x)$ are in general *not* square integrable and hence the name for the method.

Since the ground state wave function vanishes only at the end points of the boundary[1] and the nodal points of the wave functions of the excited states shift upon turning on the perturbation, the *only* choice for x_0 consistent with the boundary conditions (7) is $x_0 = \infty$. In a practical numerical calculation, which is always carried out in between finite ranges, x_0 is assigned an arbitrarily large but finite value. But as x_0 approaches infinity, both $\psi_n(0, x_0)$ and $\psi_n(1, x_0)$ diverge, and a regularization process is needed to make sense of Eq. (6).

In the form of Eq. (1), taking into account of the advantage of its similarity in form to the first order equation, $\psi_n(\alpha, x)$ can easily be solved, say, using the Dalgarno–Lewis method [3] or logarithmic perturbation method [4,5] to obtain,

$$\psi_n(\alpha, x) = -\psi_0(x) \int_b^x dy \, \frac{1}{\psi_0^2(y)} \int_a^y dz \, (\alpha - \tilde{V}_n) \psi_0^2(z), \tag{8}$$

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[1]For purpose of illustration, we consider QM on a half line $[0, \infty)$.

where a and b are appropriate constants to satisfy the boundary conditions, in agreement with the results of GR.

From Eq. (8), one recovers the universal functions $F(x)$ (given as Eq. (15) in Ref. [2])

$$F(x) = -\psi_0(x) \int_b^x dy \, \frac{1}{\psi_0^2(y)} \int_a^y dz \, V(z) \psi_0^2(z). \tag{9}$$

Together with Eq. (6), one sees that the n-th order perturbation energy E_n is given by

$$E_n = \frac{J(\tilde{V}_n, x_0)}{J(1, x_0)}, \tag{10}$$

where the functional $J(V, x)$ is given by

$$J(V, x) \equiv \int_0^x dy \, \frac{1}{\psi_0^2(y)} \int_0^y dz \, V(z) \psi_0^2(z). \tag{11}$$

and the boundary condition at the endpoints has been taken care of appropriately.

Next, we would like to point out that at least in the example of the ground state of the x^4 anharmonic oscillator, the expansion of E_n in Eq. (10) can be ill-defined because both the numerator and the denominator diverge as $x_0 \to \infty$. This can be easily seen by combining the well-known results that $\tilde{V}_n$ is of polynomial form in the Bender–Wu [6] x^4 anharmonic oscillator and the mean value theorem.

From the form of Eq. (11), one does *not* expect *a priori* that in the limit $x_0 \to \infty$, the ratio $J(\tilde{V}_n, x_0)/J(1, x_0)$ becomes finite and x_0 independent even though numerically this comes out to be so. Hence to make sense out of Eqs. (10) and (11), a regularization procedure is in order. One can justify the numerical result obtained by assigning an arbitrarily large but finite value to x_0 only after the result is regularized and the limit is proven to exist.

The regularization procedure being proposed here is similar to the one we previously used in the extension of logarithmic perturbation theory to excited bound states in one dimension by appropriately mixing in the ghost state [7]. For the zeroth order solution (unperturbed state), instead of using the square integrable eigenstate wave function ψ_0, we can mix in the non-square-integrable ghost state χ_0 by defining

$$\Psi_0(x) \equiv \psi_0(x) + i\sigma\chi_0(x), \tag{12a}$$

$$\rho(x) \equiv \Psi_0^2(x). \tag{12b}$$

and

$$J_\sigma[S] \equiv \int_0^\infty dy\, \frac{1}{\rho(y)} \int_0^y dz\, \rho(z) S(z). \tag{12c}$$

Note that in Eq. (12b), $\rho(x)$ is the ordinary square of $\Psi_0(x)$, not $|\Psi_0(x)|^2$. Then Eq. (10) can be rewritten on firm mathematical ground as

$$E_n = \lim_{\sigma\to 0} \frac{J_\sigma[\tilde{V}_n]}{J_\sigma[1]} \tag{13}$$

Now, we can show that the limit in Eq. (13) is the well-defined. This follows from [7]

$$\begin{aligned} J_\sigma[S] &= \frac{i}{\sigma} \int_0^\infty dy\, \Psi_0(y)\psi_0(y)S(y) \\ &= \frac{i}{\sigma} \int_0^\infty dy\, \psi_0^2(y)S(y) + \cdots, \end{aligned} \tag{14}$$

where $\cdots$ is a σ independent term. Upon substituting Eq. (14) into Eq. (13), we recover

$$E_n = \frac{\int_0^\infty dy\, \psi_0^2(y)\tilde{V}_n(y)}{\int_0^\infty dy\, \psi_0^2(y)} = \int_0^\infty dy\, \psi_0(y)V_1(y)\psi_{n-1}(y) \tag{15}$$

which is the ordinary QM result upon using Eq. (3) and (4). Hence, we have provided a rigorous justification of the SC method. It is interesting to note that we have also utilized non-square-integrable functions through the ghost state mixing.

To sum up, we see that the SC method correctly gives the perturbation energies, but as a ratio of two divergent quantities. We have regularized it through ghost state mixing and our final result is independent of the mixing parameter σ. It is only after establishing the existence of the limit in Eq. (13) that we can accept the numerical convergence in Eq. (10) advocated in the SC method.

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