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COMMENT

Reply to comments on 'A new efficient method for calculating perturbation energies using functions which are not quadratically integrable'

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Abstract. In a previous paper (Skála and Čížek 1996) a new approach to calculating perturbation energies of bound states based on the use of functions which are not quadratically integrable was suggested. This method has been analysed in a comment by Guardiola and Ros (1996). The present comment is the reply to this previous comment. The aim is to give a simple and straightforward proof of the method and clarify some other points important for its application.

Following [1] and [2], the Hamiltonian, wavefunction and energy in the perturbation theory are assumed in the usual forms

$$H = H_0 + \lambda H_1 \tag{1}$$

$$\psi = \psi_0 + \lambda\psi_1 + \lambda^2\psi_2 + \cdots \tag{2}$$

and

$$E = E_0 + \lambda E_1 + \lambda^2 E_2 + \cdots. \tag{3}$$

Using these assumptions in the Schrödinger equation $H\psi = E\psi$, the well known equations for E_n and ψ_n are obtained:

$$H_0\psi_0 = E_0\psi_0 \tag{4}$$

and

$$H_0\psi_n + H_1\psi_{n-1} = \sum_{i=0}^{n} E_i\psi_{n-i} \qquad n = 1, 2, \ldots. \tag{5}$$

The perturbation energies E_n in this equation are determined from the corresponding boundary conditions.

Assuming the validity of the normalization and orthogonality conditions

$$\langle\psi_0|\psi_n\rangle = \delta_{0,n} \qquad n = 0, 1, \ldots \tag{6}$$

the well known formula for E_n

$$E_n = \langle\psi_0|H_1|\psi_{n-1}\rangle \qquad n = 1, 2, \ldots \tag{7}$$

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can be easily derived.

In [1], we suggested another formula for the perturbation energy

$$E_n = -\frac{\psi_n(0, x_0)}{F(x_0)} \qquad n = 1, 2, \ldots \tag{8}$$

in which the validity of equation (6) is not assumed. Here, $\psi_n(E_n, x)$ denotes the solution of equation (5) for the energy E_n and x_0 is the point where the boundary conditions

$$\psi_n(x_0) = 0 \qquad n = 0, 1, \ldots \tag{9}$$

are applied. $F(x)$ is a universal function which can be calculated from the equation

$$F(x) = \psi_1(1, x) - \psi_1(0, x). \tag{10}$$

We note that E_n in $\psi_n(E_n, x)$ is not the value of the perturbation energy, but a parameter which is used during the integration of equation (5) for a given n. In consequence, functions $\psi_n(E_n, x)$ are not in general quadratically integrable. It applies also for $E_n = 1$ and $E_n = 0$.

Equation (8) is a very simple and interesting result showing that functions which are not quadratically integrable can be used for the calculation of the perturbation energies of quadratically integrable states.

In [1], detailed discussion of the validity of equations (8) and (10) was not given. This has been noted in [2] and a rather complicated proof of these equations has been elaborated. Discussion of the boundary conditions in the numerical solution of equation (5) has not been performed in [1] and [2]. The aim of this comment is to show that equations (8) and (10) follow very simply from equation (5) if these conditions are taken in the usual form. We would also like to comment on some remarks regarding the numerical properties of our method.

Now we assume that E_i and $\psi_i(x)$, $i = 0, \ldots, n-1$ are the correct perturbation energies and wavefunctions.

Following [2], we denote

$$\sum_{i=1}^{n-1} E_i \psi_{n-i}(x) - H_1 \psi_{n-1}(x) = \mathcal{F}(x). \tag{11}$$

Then, equation (5) becomes

$$(H_0 - E_0)\psi_n(E_n, x) = E_n \psi_0(x) + \mathcal{F}(x) \qquad n = 1, 2, \ldots. \tag{12}$$

Subtracting this equation for a general value of the parameter E_n and for $E_n = 0$ we get

$$(H_0 - E_0)(\psi_n(E_n, x) - \psi_n(0, x)) = E_n \psi_0(x). \tag{13}$$

For $E_n = 1$, this equation yields

$$(H_0 - E_0)(\psi_n(1, x) - \psi_n(0, x)) = \psi_0(x). \tag{14}$$

Using the last expression for $\psi_0(x)$ in equation (13) we get

$$(H_0 - E_0)(\psi_n(E_n, x) - \psi_n(0, x)) = E_n(H_0 - E_0)(\psi_n(1, x) - \psi_n(0, x)). \tag{15}$$

We see from this equation that, in general,

$$\psi_n(E_n, x) - \psi_n(0, x) = E_n(\psi_n(1, x) - \psi_n(0, x)) + G_n(E_n)\psi_0(x) \tag{16}$$

where $G_n(E_n)$ is a function of E_n.

To determine $G_n(E_n)$, we assume the same boundary conditions for ψ_n as in the usual numerical solution of equation (5). We suppose that the integration of equation (5) is performed on a finite but sufficiently large interval $\langle x_s, x_0 \rangle$. Here, x_s ($x_s < x_0$) is the

starting point of the integration and x_0 is the final point where the boundary conditions (9) are applied. At the starting point x_s, we keep constant the value of the wavefunction $\psi_n(E_n, x_s)$ for all the values of the parameter E_n

$$\psi_n(E_n, x_s) = c_n \qquad n = 0, 1, \ldots . \tag{17}$$

Here, c_n is a small number different from zero. To define $\psi_n(E_n, x)$ uniquely, we make similar assumption also about its derivative

$$\left.\frac{\partial \psi_n(E_n, x)}{\partial x}\right|_{x=x_s} = d_n, \; n = 0, 1, \ldots \tag{18}$$

where d_n is a small number or zero. Values of the constants c_n and d_n are not critical. The value of the perturbation energy E_n is determined by the boundary condition (9).

Using the boundary condition (17) in equation (16) we get

$$G_n(E_n)\psi_0(E_0, x_s) = 0. \tag{19}$$

Taking into account the fact that $\psi_0(E_0, x_s) = c_0 \neq 0$ we see that

$$G_n(E_n) = 0 \tag{20}$$

and

$$\psi_n(E_n, x) - \psi_n(0, x) = E_n(\psi_n(1, x) - \psi_n(0, x)). \tag{21}$$

Let us assume now that E_n is the perturbation energy determined by the boundary condition $\psi_n(E_n, x_0) = 0$. Then, equation (21) gives for $x = x_0$

$$E_n = -\frac{\psi_n(0, x_0)}{\psi_n(1, x_0) - \psi_n(0, x_0)} \qquad n = 1, 2, \ldots . \tag{22}$$

Writing equation (14) for general n and for $n = 1$ we get the result similar to equation (16)

$$\psi_n(1, x) - \psi_n(0, x) = \psi_1(1, x) - \psi_1(0, x) + g_n\psi_0(x) \tag{23}$$

where g_n is a constant. It is obvious that $g_n = 0$ for the same reason as $G_n(E_n) = 0$ and

$$\psi_n(1, x) - \psi_n(0, x) = \psi_1(1, x) - \psi_1(0, x). \tag{24}$$

We see that the difference $\psi_n(1, x) - \psi_n(0, x)$ is a universal function of x denoted as $F(x)$ in [1]

$$\psi_n(1, x) - \psi_n(0, x) = F(x) \qquad n = 1, 2, \ldots . \tag{25}$$

With this function, equation (22) can be written in the form of equation (8). Equation (11) of [1]

$$\frac{\partial \psi_n(E_n, x)}{\partial E_n} = F(x) \tag{26}$$

is a trivial consequence of equations (21) and (25).

We note that the perturbation H_1 does not appear in (13). Therefore, $F(x)$ is a universal function not only for all orders $n = 1, 2, \ldots$ but also for all the perturbations H_1 assuming that the zero-order Hamiltonian H_0 does not change and the boundary conditions for ψ_n have the form of equations (9), (17) and (18).

During our proof of equation (8), the validity of the normalization and orthogonality conditions (6) was not assumed. Therefore, equation (8) is more general than equation (7). It is remarkable that, in contrast to the variational methods or usual versions of the perturbation theory such as (7), no matrix elements have to be calculated in equation (8). To determine E_n from this equation, only one function value $\psi_n(0, x_0)$ and $F(x_0)$ must be known.

Since the validity of the normalization and orthogonality conditions (6) is not required in our method, the wavefunctions ψ_n calculated numerically from equation (5) can in general contain an arbitrary component of ψ_0. It is obvious that it leads to the renormalization of the ψ_0 component in the resulting wavefunction ψ. If required, the orthogonality conditions (6) can be obeyed by the usual orthogonalization scheme.

Finally, we note that the calculation of eigenfunctions for eigenvalues taken as parameters is a part of standard algorithms for the calculation of eigenvalues of differential equations. In these algorithms, differential equations are numerically integrated and estimates of the eigenvalues are changed until the boundary conditions are obeyed. Such 'shooting' methods represent a standard numerical procedure and have no special problems with instabilities and overflows. In [1] and in this comment, we have discussed a special case of differential equations, namely, the perturbation equations. From this point of view, the remark in [2], according to which the method using functions that are not normalizable is prone to instabilities and overflows, seems to be out of place.

Finally, let us repeat [1] that the two most important applications are the strong coupling perturbation theory [3–11] as well as a rigorous mathematical theory of the upper and lower bounds [12] which is more effective than the inner projection technique [13].

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