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COMMENT

Comment on the letter 'A new efficient method for calculating perturbation energies using functions which are not quadratically integrable' by L Skála and J Čížek

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Abstract. We suggest that the recent numerical-integration perturbative approach to bound states as proposed by Skála and Čížek may be generalized via its renormalizations.

1. Introduction

The phenomenological Schrödinger bound-state problem

$$\left[-\frac{d^2}{dx^2}+\frac{\ell(\ell+1)}{x^2}+V(x)\right]\psi(x)=\varepsilon\psi(x) \qquad \psi(x_0)=0 \qquad x_0\to\infty \tag{1}$$

with a regular potential $V(x)$ in one or three dimensions (i.e. with parity $\ell=-1,\ 0$ or angular momentum $\ell=0,\ 1,\ \ldots$, respectively) is currently being solved by a shooting method [1]. Basically, at a finite but sufficiently large $x_0\gg 1$, a trial choice of the energy ε and of an initialization regular in the origin,

$$\psi(x)\approx c\,x^{\ell+1} \qquad x\approx 0 \qquad c\neq 0 \tag{2}$$

enables us to integrate equation (1) numerically. At $\varepsilon\neq\varepsilon^{(\text{physical})}$, the right-most nodal zero x_r of the resulting numerical $\psi(\varepsilon,x)$ does not lie at its correct position x_0 of course. Fortunately, due to the well known oscillation rule

$$\begin{aligned}&\varepsilon^{(\text{improved})}<\varepsilon &&\text{for } x_r<x_0\\ &\varepsilon^{(\text{improved})}>\varepsilon &&\text{for } x_r>x_0\end{aligned} \tag{3}$$

one may improve the energy guess iteratively. Recently, a generalization of this scheme to perturbed systems

$$\begin{aligned}&H\psi(x)=E\psi(x)\\ &H=H_0+\lambda H_1\ (+\lambda^2H_2+\cdots)\\ &E=E_0+\lambda E_1+\lambda^2E_2+\cdots\\ &\psi(x)=\psi_0(x)+\lambda\ \psi_1(x)+\lambda^2\psi_2(x)+\cdots\end{aligned} \tag{4}$$

with the exactly solvable/solved zeroth-order problem

$$(H_0-E_0)\ \psi_0(x)=0 \qquad \psi_0(x_0)=0 \qquad x_0\gg 1 \tag{5}$$

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has been proposed by Skála and Čížek (SČ, [2]). Their method is based on a replacement of the separate $O(\lambda^n)$ Rayleigh–Schrödinger (RS) components of equation (4):

$$(H_0 - E_0)\ \psi_n(x) + (H_1 - E_1)\ \psi_{n-1}(x) + \cdots + (H_n - E_n)\ \psi_0(x) = 0 \qquad n = 1, 2, \ldots \tag{6}$$

by the numerically more tractable set of equations

$$(H_0 - E_0)\ \varphi_n(\varepsilon, x) + (H_1 - E_1)\ \psi_{n-1}(x) + \cdots + (H_{n-1} - E_{n-1})\ \psi_1(x) + H_n\psi_0(x) = \varepsilon\ \psi_0(x) \tag{7}$$

with the same initial boundary condition (2) as above, namely

$$\varphi_n(\varepsilon, x) \approx c\, x^{\ell+1} \qquad x \approx 0 \qquad c \neq 0\,. \tag{8}$$

Here, at each perturbation order $n = 1, 2, \ldots$, the asymptotic boundary condition has been relaxed, $\varphi_n(\varepsilon, x_0) \neq 0$ and $\varepsilon \neq E_n$. As a consequence, one may differentiate equations (7) with respect to the variable ε:

$$(H_0 - E_0)\partial_\varepsilon \varphi_n(\varepsilon, x) = \psi_0(x)\,. \tag{9}$$

From this equation, Skála and Čížek inferred that the ε-dependence of $\varphi_n(\varepsilon, x)$ must be linear and n-independent,

$$\varphi_n(\varepsilon, x) = \varphi_n(0, x) + \varepsilon\, F(x) \tag{10}$$

(cf [2, equation (12)]). Strictly speaking, such a conclusion is invalid: we may always renormalize

$$F(x) \to F(x) + f_0\psi_0(x) + \varepsilon\, f_1\psi_0(x) + \varepsilon^2 f_2\psi_0(x) + \cdots\,. \tag{11}$$

This puzzle inspired the discussion that follows.

2. Renormalization

Let us fix the parameter c in the initialization (8). Equations (7) then define the regular solutions $\varphi_n^{[c]}(\varepsilon, x)$ at any ε and n in principle. At a different value of c, we get a 'renormalized' solution

$$\varphi_n^{[c_R]}(\varepsilon, x) = \varphi_n^{[c]}(\varepsilon, x) + d_n(\varepsilon)\, \varphi_0^{[c]}(E_0, x) \tag{12}$$

(quotation marks indicate that the normalization integrals $\int_0^{x_0}\cdots$ might diverge in the $x_0 \to \infty$ limit) and, of course, c_R may be both n- and ε-dependent.

2.1. The SČ quasi-normalization

Once we accept the SČ linearity constraint in its fixed-c form (10) simply as a certain pseudo-inversion *postulate*

$$\varphi_n^{[c]}(\varepsilon, x) = \varphi_n^{[c]}(0, x) + \varepsilon\, F(x) \qquad n = 0, 1, \ldots \tag{13}$$

we may define the factor $F(x)$ directly, by equation (9):

$$(H_0 - E_0)\ F(x) = \psi_0(x) \tag{14}$$

with a modified near-the-threshold initialization

$$F(x) = O(x^{\ell+2}) \qquad |x| \ll 1\,. \tag{15}$$

Thus, our present notation clarifies the puzzle (11) as reflecting the particular SČ choice of normalization

$$d_0^{(\mathrm{S\check{C}})} = d_1^{(\mathrm{S\check{C}})} = d_2^{(\mathrm{S\check{C}})} = \cdots = 0\,. \tag{16}$$

As a byproduct, our analysis enables us to simplify the SČ algorithm itself. During the evaluation of the first-order energy

$$E_1 = -\varphi_1(0, x_0)/F(x_0) \qquad F(x_0) = \varphi_1(1, x_0) - \varphi_1(0, x_0) \tag{17}$$

defined via the double integration of the $n = 1$ equation (7)

$$(H_0 - E_0)\ \varphi_1^{[c]}(\varepsilon, x) + H_1\psi_0(x) = \varepsilon\ \psi_0(x) \tag{18}$$

at $\varepsilon = 0$ and at $\varepsilon = 1$ [2], one may replace the latter step by the integration of equations (14) and (15). This is a slightly simpler task: the H_1 perturbation term is absent.

2.2. The standard RS renormalization

The renormalization ambiguity (12), i.e. in the light of (8), the freedom

$$c \to c_{\mathrm{R}}(\varepsilon, n) = c \times [1 + d_n(\varepsilon)] \qquad n = 0, 1, \ldots \tag{19}$$

is usually suppressed, in the current textbook spirit [3], by the RS requirements of normalization and orthogonality,

$$\langle\psi_0|\ \psi_0\rangle = 1 \qquad \langle\psi_0|\ \psi_1\rangle = \langle\psi_0|\ \psi_2\rangle = \cdots = 0. \tag{20}$$

This determines the particular RS sequence of d's:

$$d_0^{(RS)}(E_0) = -1 + \left[\int_0^{x_0} |\varphi_0^{[c]}(E_0, t)|^2\ \mathrm{d}t\right]^{-1} \tag{21}$$

$$d_n^{(RS)}(E_n) = -\frac{\int_0^{x_0} \varphi_0^{[c]*}(E_0, \tau)\varphi_n^{[c]}(E_n, \tau)\ \mathrm{d}\tau}{\int_0^{x_0} |\varphi_0^{[c]}(E_0, t)|^2\ \mathrm{d}t} \qquad n = 1, 2, \ldots \tag{22}$$

at the physical ε's. Such an 'on-the-energy-shell' constraint still admits a virtually arbitrary ε-dependence. This is not surprising: within the textbook RS framework, we are not expected to leave the space of quadratically integrable functions.

3. A $c \longrightarrow 0$ renormalization

After a return to a broader space of functions, the RS-inspired possibility of an n-dependence of the initial slopes $c_{\mathrm{R}} = c_{\mathrm{R}}(n)$ of the renormalized regular solutions $\varphi_n^{[c_{\mathrm{R}}]}(\varepsilon, x)$ near the origin opens a broad new area of modifications of the SČ algorithm. Some of them may be expected to exhibit a close relationship to various perturbation theories which use integrations over the coordinates [4]. This will not be analysed here in any greater detail; let us just mention the simplest, highly degenerate (HD) possibility of letting all the higher-order c_{R}'s vanish:

$$c_{\mathrm{R}}^{(\mathrm{HD})}(n) = 0 \qquad n = 1, 2, \ldots\,. \tag{23}$$

Of course, we must keep the first, unperturbed $c_{\mathrm{R}}(0)$ non-zero, $c_{\mathrm{R}}^{(\mathrm{HD})}(0) \neq 0$; otherwise, there would not be any non-zero ψ_0 at all. For convenience, we may preserve the above RS or SČ $n = 0$ normalization convention unchanged.

Technically, the renormalized HD algorithm remains straightforward. We only have to replace the numerical initialization condition (8) by its modification which is similar to (15):

$$\varphi_n^{[0](\mathrm{HD})}(\varepsilon, x) = \mathrm{O}(x^{\ell+2}) \qquad |x| \ll 1 \qquad n = 1, 2, \ldots . \tag{24}$$

It may prove useful, e.g., within the so-called Hill-determinant method [5] and its various perturbative modifications [6]. In this context, the SČ-like linearity assumption

$$\varphi_n^{[0](\mathrm{HD})}(\varepsilon, x) = \varphi_n^{[0](\mathrm{HD})}(0, x) + \varepsilon\, F(x) \qquad n = 0, 1, \ldots \tag{25}$$

acquires a less sophisticated interpretation as a certain close parallel of the standard RS model-space-projection recipe for a decomposition of a wavefunction in a certain non-orthogonalized expansion basis, with $F(x)$ and $\varphi_n^{[0](\mathrm{HD})}(0, x)$ playing the role of its internal and external components, respectively [6, 7].

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