New perturbation method
with the matching of wave functions

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Abstract
We propose a new approach to the Rayleigh-Schrödinger perturbation expansions of
bound states in quantum mechanics. We are inspired by the enormous flexibility of
solvable interactions with several \((N)\) discontinuities. Their standard matching solu-
tion is modified and transferred in perturbation regime. We employ the \textit{global}
renormalization freedom of the \textit{local} wave functions and derive a compact \(N\text{–}d\)imensional
matrix formula for corrections. In applications, our recipe is shown non-numerical
for all polynomial perturbations of any piece-wise constant zero order potential.

[KEYWORDS]

[Matching method] for [Rayleigh-Schrödinger corrections] to [bound states] within
[perturbation theory (using) symbolic manipulations] applied to [piece-wise constant
potentials (with) polynomial perturbations].
1 Introduction

Rayleigh-Schrödinger perturbation theory [1] leads to several popular and efficient numerical approximation methods [2]. Its construction of observables may also prove inspiring in the more abstract analysis of their coupling dependence [3]. The latter role of the perturbative power series ansatzs has already been emphasized in the classical monograph by Morse and Feshbach [4]. Their presentation of the Rayleigh-Schrödinger formalism contemplates any potential $V(r) = V^{(0)}(r) + \lambda V^{(1)}(r)$ as defined on a trivial square-well background $V^{(0)}(r)$.

In the late sixties the “mainstream” attention has been shifted to analytic $V^{(0)}(r)$. People have noticed that a suitable normalization leads to five-term recurrences and to an enormous simplification of the construction of the anharmonic oscillators with $V^{(1)}(r) \sim r^4$ etc. The history has been reviewed, e.g., by Simon [6].

An unpleasant obstacle to a broader applicability of perturbative solutions formed by the power series in $\lambda$ is definitely the narrow variability of the available analytic zero order approximations. In three dimensions Newton [7] only lists square well $V^{(0)}(r) \sim (r/L)^p$, $p \to \infty$, harmonic well $V^{(0)}(r) \sim (r/L)^2$, Coulomb field $V^{(0)}(r) \sim (r/L)^{-1}$ and a rather exotic strongly singular $V^{(0)}(r) \sim (r/L)^{-4}$.

The non-analytic square well seems tedious in comparison but in the present paper we still return to discontinuous $V^{(0)}(r)$. A new version of the Rayleigh-Schrödinger method will be proposed. We shall argue that an appropriate “optimal” normalization is equally well able to simplify many models containing $N$ discontinuities in a way which enhances significantly the flexibility of the above-mentioned Morse-Feshbach single-well example.

Our conjecture is based on several technical ingredients. Firstly, we imagine
that the contemporary computers shift the borderlines of feasibility of the initial zero order constructions. In this sense the standard solvable square well may easily be complemented not only by its textbook modification of finite depth [3] but by virtually any piece-wise constant potential $V^{(0)}(r)$. This is discussed in Section 2. For definitness we pick up there the $s$-wave ($\ell = 0$) rectangular or step-shaped example

$$V^{(0)}_{(N)}(r) = \begin{cases} 
\infty, & r \in (-\infty, L_0) \cup (L_{N+1}, \infty) \\
H_j, & r \in (L_j, L_{j+1}), 
\end{cases} \quad j = 0, 1, \ldots, N \tag{1}$$

with impenetrable outer barriers $H_{N+1} = \infty$ and $H_{-1} = \infty$ and with $N$ discontinuities and $L_0 \geq 0$. These specifications are just convenient and could easily be altered.

The study of perturbations of the more and more complicated solvable potentials (1) reveals that the standard use of an unperturbed basis may become prohibitively cumbersome. The evaluation of all the necessary Rayleigh-Schrödinger overlap integrals does not seem rewarded by the resulting series

$$\psi(x) = \psi^{(0)}(x) + \lambda \psi^{(1)}(x) + \lambda^2 \psi^{(2)}(x) + \ldots, \quad E = E^{(0)} + \lambda E^{(1)} + \lambda^2 E^{(2)} + \ldots. \quad (2)$$

A simpler recipe is asked for. In section 3 we propose, therefore, a new approach to corrections which circumvents the use of integrals. We shall see how it combines the continuity of our Schrödinger differential equation on certain finite intervals with an ease of their mutual matching.

The formal appeal of our new technique lies in its unexpectedly coherent combination of the matching of perturbed wave functions $\psi^{(k)}(r)$ with a “hidden” freedom of their normalization. The idea transcends its present application and makes the formalism quite universal. Our matching of perturbation corrections may be under-
stood as a useful alternative to the standard textbook recipe even in applications to
smooth potentials. This is discussed in the last Section 4.

2 Matching method in zero order

We usually expect that a split of a given potential $V(x)$ into a dominant part $V^{(0)}(x)$
and its perturbation $\lambda V^{(1)}(x)$ simplifies our Schrödinger equation in its unperturbed
limit $\lambda \to 0$. Potentials $V^{(0)}(x)$ are predominantly chosen as harmonic oscillators.
The more complicated shapes of $V(x)$ can hardly be treated by perturbation expansions without resort to their discontinuous approximants.

2.1 The piece-wise constant unperturbed potentials

The first non-trivial $s$–wave step-like example (II) with $N = 1$, gauge $H_0 = 0$, energy
$E = \beta^2$, step $H_1 = \beta^2 - \gamma^2$ and abbreviations $L_0 = 0$, $L_1 = P$, $L_2 = Q$ possesses the
trivial wave functions

$$
\psi^{(0)}(x) = \begin{cases} 
\beta^{-1} \sin \beta x, & x \in (0, P) \\
\mathcal{N} \gamma^{-1} \sin \gamma(x - Q), & x \in (P, Q) 
\end{cases}
$$

Their matching at $P$ fixes $\mathcal{N}$ and defines the energies as roots of the elementary
trigonometric equation

$$
\gamma \tan \beta P = \beta \tan \gamma(P - Q).
$$

In the less common $N = 2$ example with $L_3 = R$ let us abbreviate $E = \beta^2$, $\alpha^2 = H_1 - \beta^2$ and $\gamma^2 = \beta^2 - H_2$ and admit the complex $\alpha$, $\beta$ and $\gamma$ in

$$
\psi^{(0)}(x) = \begin{cases} 
\beta^{-1} \sin \beta x, & x \in (0, P) \\
\alpha^{-1} \left( c_1 e^{\alpha(x - P)} - c_2 e^{-\alpha(x - P)} \right), & x \in (P, Q) \\
\mathcal{N} \gamma^{-1} \sin \gamma(x - Q), & x \in (Q, R) 
\end{cases}
$$
In terms of $B = \beta P$, $C = \gamma (Q - R)$, $A = \arctg(\alpha / \beta)$ and $D = \arctg(\alpha / \gamma)$ the spectrum follows from the similar matching condition

$$e^{\alpha (Q - P)} \cos(B - A) \cos(C + D) - e^{-\alpha (Q - P)} \cos(B + A) \cos(C - D) = 0. \quad (3)$$

The graphical localization of its zeros is sampled in Figure 1 where we have chosen $P = 1$, $Q = 2$ and $R = \pi$. With the double-well choice of $H_2 = 0$ the Figure displays our double-well secular determinant at the four different heights of its central barrier. In principle, these curves range from zero up to the maximal $k = \beta = \sqrt{H_1}$ where they turn purely imaginary. Our picture shows just a small vicinity of the quasi-degenerate doublet of the two lowest energies. Due to the asymmetry of $V^{(0)}(x)$ their split only very weakly depends on the repulsive central core.

### 2.2 Trigonometric symbolic manipulations

After we move to the higher integers $N$ the assistance of a computer becomes welcome. For example, the choice of $N = 4$ may mimic a double tunneling. With $H_0 = H_2 = H_4 = 0$ and $H_1 = H_3 = H > 0$, at the energy $E = \kappa^2 = H \cos \alpha$ and with abbreviations $L_4 = S$, $L_5 = T$, $\delta = \sqrt{H - E} \equiv \sqrt{H} \sin \alpha > 0$ and

$$F(\alpha) = \sin[(R - Q) \kappa(\alpha)] \cos[(T - S) \kappa(\alpha) + \alpha] \cos[P \kappa(\alpha) - \alpha],$$

$$G(\alpha) = \sin[2\alpha - (R - Q) \kappa(\alpha)] \cos[(T - S) \kappa(\alpha) - \alpha] \cos[P \kappa(\alpha) - \alpha]$$

we derive the secular equation

$$e^{(Q - P)\delta} [F(\alpha)e^{(S - R)\delta} + G(\alpha)e^{-(S - R)\delta}] = e^{-(Q - P)\delta} [F(-\alpha)e^{(S - R)\delta} + G(-\alpha)e^{-(S - R)\delta}].$$
It is fairly transparent. In our last example with \( N = 6 \) the triplet of barriers in

\[
V_{(QW)}(x) = \begin{cases} 
0, & x \in (0, P) \cup (Q, R) \cup (S, T) \cup (U, W) \\
H, & x \in (P, Q) \cup (R, S) \cup (T, U) \\
\infty, & x \in (-\infty, 0) \cup (W, \infty)
\end{cases}
\]

requires similar strategy. With the four auxiliary functions

\[
F_1 = \cos(P \kappa + \alpha) \sin[(R - Q) \kappa + 2 \alpha] \sin[(T - S) \kappa + 2 \alpha] \cos[(W - U) \kappa + \alpha], \\
F_2 = \cos(P \kappa + \alpha) \sin[(R - Q) \kappa + 2 \alpha] \sin[(T - S) \kappa] \cos[(W - U) \kappa - \alpha], \\
F_3 = \cos(P \kappa + \alpha) \sin[(R - Q) \kappa] \sin[(T - S) \kappa] \cos[(W - U) \kappa + \alpha], \\
F_4 = \cos(P \kappa + \alpha) \sin[(R - Q) \kappa] \sin[(T - S) \kappa - 2 \alpha] \cos[(W - U) \kappa - \alpha]
\]

of \( \alpha \) and \( \kappa = \kappa(\alpha) = \kappa(-\alpha) = \sqrt{H} \cos \alpha \equiv \sqrt{E} > 0 \) and with the same \( \delta = |\delta| = \sqrt{H - E} \equiv \sqrt{H} \sin \alpha > 0 \) as above, the exact secular equation is

\[
\begin{align*}
-F_1(\alpha) e^{2(P + R + T) \delta(\alpha)} + F_2(\alpha) e^{2(P + R + U) \delta(\alpha)} + F_3(\alpha) e^{2(P + S + T) \delta(\alpha)} \\
- F_4(\alpha) e^{2(P + S + U) \delta(\alpha)} + F_1(-\alpha) e^{2(Q + S + U) \delta(\alpha)} - F_2(-\alpha) e^{2(Q + S + T) \delta(\alpha)} \\
- F_3(-\alpha) e^{2(Q + R + U) \delta(\alpha)} + F_4(-\alpha) e^{2(Q + R + T) \delta(\alpha)} e^{[(P - Q - R - S - T - U) \delta(\alpha)]} = 0.
\end{align*}
\]

The study of the other similar systems may be guided by this experience. The longer ansatzs remain tractable by computerized trigonometric manipulations.

### 2.3 The general matching recipe

Any Schrödinger bound state problem with a piece-wise constant potential is exactly solvable on each sub-interval \((L_j, L_{j+1})\). Its two independent solutions are just the (trigonometric or hyperbolic) sines \( S_j^+(x) \) and cosines \( C_j^+(x) \) determined in a unique way by the left initial conditions,

\[
C_j^+(x) \bigg|_{x=L_j} = 1, \quad \partial_x C_j^+(x) \bigg|_{x=L_j} = 0, \\
S_j^+(x) \bigg|_{x=L_j} = 0, \quad \partial_x S_j^+(x) \bigg|_{x=L_j} = 1. \tag{4}
\]
They define the general solution simply as a superposition

$$\psi^{(0)}(x) = c^{(+)}(j) C^{(+)}_j(x) + d^{(+)}(j) S^{(+)}_j(x), \quad x \in (L_j, L_{j+1}), \quad j = 0, 1, \ldots, N. \quad (5)$$

In the light of the obvious symmetry of our global problem on \((L_0, L_{N+1})\), one can equally well employ the alternative ansatz

$$\psi^{(0)}(x) = c^{(-)}(j + 1) C^{(-)}_{j+1}(x) + d^{(-)}(j + 1) S^{(-)}_{j+1}(x), \quad x \in (L_j, L_{j+1}), \quad (6)$$

with the \((-\text{)}\)-superscripted basis defined by the right initial conditions

$$C^{(-)}_{j+1}(x) \bigg|_{x=L_{j+1}} = 1, \quad \partial_x C^{(-)}_{j+1}(x) \bigg|_{x=L_{j+1}} = 0,$$
$$S^{(-)}_{j+1}(x) \bigg|_{x=L_{j+1}} = 0, \quad \partial_x S^{(-)}_{j+1}(x) \bigg|_{x=L_{j+1}} = 1. \quad (7)$$

We may immediately make the following two conclusions.

- The standard matching of the logarithmic derivatives at every discontinuity

  $$x = L_j$$

  finds an elementary though rigorous guarantee in the obvious rule

  $$c^{(+)}(j) = c^{(-)}(j) = c(j), \quad d^{(+)}(j) = d^{(-)}(j) = d(j), \quad j = 0, 1, \ldots, N+1.$$

  This is the first simplification of our two alternative formulae \((5)\) and \((6)\) for wave functions.

- In each interval \((L_j, L_{j+1})\), any two-point boundary conditions \(\psi^{(0)}(L_j) = c(j)\), \(\psi^{(0)}(L_{j+1}) = c(j + 1)\) make the solution unique. This statement is equivalent to the two simple rules

  $$c(j) = c(j + 1) C^{(-)}_{j+1}(L_j) + d(j + 1) S^{(-)}_{j+1}(L_j), \quad \text{and}$$
$$c(j + 1) = c(j) C^{(+)}_j(L_{j+1}) + d(j) S^{(+)}_j(L_{j+1}) \quad (8)$$

where, of course, \(c(0) = 0\) and \(c(N + 1) = 0\) and \(j = 0, 1, \ldots, N\). We may summarize that as a net result of our construction we have to solve just the \(2N + 2\) homogeneous and linear algebraic equations for the \(2N + 2\) unknown parameters.
In a marginal comment let us also note that our choice of \( c(0) = 0 \) and \( c(N + 1) = 0 \) is dictated by the underlying physics which requires the most common Dirichlet form of the outer boundary conditions. In a more formal approach one could also keep in mind the possible alternative choices of the Neumann conditions \( d(0) = 0 \) and \( d(N + 1) = 0 \) or of the important periodic option for \( c(0) = c(N + 1) \) and \( d(0) = d(N + 1) \) etc. Unfortunately, their detailed study would already lead us far beyond our present task.

### 2.4 Piece-wise polynomial unperturbed potentials

We have seen that the practical use of our nonstandard matching recipe (8) is a well defined numerical problem. Its solution requires just the knowledge of the independent sine and cosine solutions and an evaluation of their values at all the points of the discontinuities \( x = L_j \). It is important to note that our rigorous matching recipe works with the two independent bases. This enables us to avoid the more usual but, sometimes, less comfortable construction of the derivatives of the basis. In this sense, a slight generalization of this recipe may be easily applied to all the zero-order problems

\[
- \frac{d^2}{dx^2} \psi^{(0)}(x) + V^{(0)}(x) \psi^{(0)}(x) = E^{(0)} \psi^{(0)}(x) \tag{9}
\]

with any piece-wise polynomial discontinuous potential

\[
V^{(0)}(x^{\pm}) \sim \sum_{l=0}^{p \pm j} \int_{l}^{(x^{\pm} - L_j)} w^{\pm}_{l}(j) (x^{\pm} - L_j), \quad x^{+} \geq L_j, \quad x^{-} \leq L_j. \tag{10}
\]

Locally (i.e., within the “double” intervals \( \mathcal{J}_j = (L_{j-1}, L_{j+1}) \) such that \( L_{-1} \equiv L_0 \) and \( L_{N+2} \equiv L_{N+1} \) we may drop the redundant argument \( j \) and superscripts \( ^{(0)} \) and search for the exact wave functions in their respective left and right Taylor series.
form

$$\psi(x^\pm) \sim \sum_{n=0}^{M} \tilde{h}_{n}^\pm(j)(x^\pm - L_j)^n, \quad M \to \infty.$$  

In a purely numerical implementation Hodgson’s tests [10] confirm the fast convergence of such a “local” recipe with \( N \to \infty \). In the present perturbation context the number of discontinuities \( x = L_j \) at \( j = (0), 1, 2, \ldots, N, (N + 1) \) is fixed and, presumably, very small, \( N = \mathcal{O}(1) \). Still, in a compactified notation which parallels our previous \( p(\pm j) = 0 \) construction we can drop the superscripts \( \pm \) and re-write our local Taylor series as superpositions

$$\psi(x) = c(j)C_j(x) + d(j)S_j(x), \quad x \in (L_{j-1}, L_{j+1}), \quad j = 0, 1, \ldots, N + 1. \quad (11)$$

Their two components \( C_j(x) = C(x) \) and \( S_j(x) = S(x) \) are independent solutions of our ordinary differential Schrödinger equation (9) again. They are uniquely determined by their respective cosine-like and sine-like behaviour at \( x = L_j \),

$$C(x)\bigg|_{x=L_j} = 1, \quad \partial_x C(x)\bigg|_{x=L_j} = 0,$$

$$S(x)\bigg|_{x=L_j} = 0, \quad \partial_x S(x)\bigg|_{x=L_j} = 1. \quad (12)$$

At the two outer boundaries \( L = L_0 \) and \( R = L_{N+1} \) the current physical conditions \( \psi(L) = \psi(R) = 0 \) acquire the most elementary form \( c(0) = 0 \) and \( c(N + 1) = 0 \) or, equivalently, \( c(1)C_1(L) + d(1)S_1(L) = 0 \) and \( c(N)C_N(R) + d(N)S_N(R) = 0 \). This parallels again the above \( p(\pm j) = 0 \) special case. The mutual matchings of the neighboring wave functions are all similar and we have the final compact set of the physical requirements

$$c(j)C_j(L_{j-1}) + d(j)S_j(L_{j-1}) = c(j - 1),$$

$$c(j)C_j(L_{j+1}) + d(j)S_j(L_{j+1}) = c(j + 1), \quad (13)$$

\( j = 1, 2, \ldots, N. \)
We have to evaluate again the $4N$ input quantities $S_j(L_{j\pm1})$ and $C_j(L_{j\pm1})$ and solve the $2N$—dimensional “secular” equation for the arbitrarily normalized coefficients in the local wave functions (11) and for the global binding energy. All our piece-wise constant illustrative examples of subsections 2.1 and 2.2 re-emerge after the choice of $p(\pm j) = 0$ in potential (10) of course.

3 Matching method for perturbations

The separate $O(\lambda^k)$ components of the perturbed Schrödinger equation have the well known non-homogeneous form

$$-\frac{d^2}{dx^2} \psi^{(k)}(x) + V^{(0)}(x) \psi^{(k)}(x) - E^{(0)} \psi^{(k)}(x) = \tau^{(k-1)}(x) + E^{(k)} \psi^{(0)}(x) \quad (14)$$

with

$$\tau^{(k-1)}(x) = -V^{(1)}(x) \psi^{(k-1)}(x) + \sum_{j=1}^{k-1} E^{(j)} \psi^{(k-1)}(x), \quad k = 1, 2, \ldots .$$

In principle, it defines the $k$—th corrections in terms of their predecessors $\psi^{(k-1)}(x)$, $\psi^{(k-2)}(x)$, . . . and $E^{(k-1)}$, $E^{(k-2)}$, . . ., “compressed” in the order-dependent right-hand side functions.

3.1 Local solutions

The matching method of subsection 2.3 does not use the (logarithmic) derivatives. This is rendered possible by a certain redundancy of our construction since domains $J_j$ overlap. We shall now apply the same strategy to the implicit definition (14) of corrections $E^{(k)} \equiv \varepsilon$ and $\psi^{(k)}(x) = \varphi(\varepsilon, \xi, x)$ split in four terms locally,

$$\psi^{(k)}_j(x) = c^{(k)}(j) C^{(k)}_j(x) + d^{(k)}(j) S^{(k)}_j(x) + \varepsilon \omega(x) + \xi^{(k)}_j \psi^{(0)}(x), \quad j = 1, 2, \ldots , N. \quad (15)$$
This is our key ansatz. Its two free parameters $\varepsilon$ and $\xi$ should facilitate the matching at the boundaries of $J_j$. Within each of these intervals and at $\varepsilon = 0$ and $\xi = 0$ the simplified order-dependent part of our non-homogeneous differential eq. (14)

$$
\left[ -\frac{d^2}{dx^2} + V^{(0)}(x) - E^{(0)} \right] \varphi(0, 0, x) = \tau^{(k-1)}(x)
$$

will define all the superpositions of the energy-independent functions $C(x)$ and $S(x)$ distinguished (and made unique) by the respective cosine- and sine-like initial conditions (12). The third auxiliary function $\omega(x) = \omega_j(x)$ will be specified as a solution of a simpler, order-independent equation

$$
\left[ -\frac{d^2}{dx^2} + V^{(0)}(x) - E^{(0)} \right] \omega(x) = \psi^{(0)}(x)
$$

with the different initial conditions

$$
\omega_j(x) \bigg|_{x=L_j} = 0, \quad \partial_x \omega_j(x) \bigg|_{x=L_j} = 0 .
$$

The fourth component $\psi^{(0)}(x)$ is known. Its contribution is weighted by the last parameter $\xi$ chosen to shift the sum $c^{(k)}(j) + d^{(k)}(j)$ by $c^{(0)}(j) + d^{(0)}(j)$ at each $j$. Assuming that $c^{(0)}(j) + d^{(0)}(j) \neq 0$ we may re-scale $c^{(k)}(j) + d^{(k)}(j) = 1$ at all $k > 0$.

The $k$– and $j$–dependent variability of $\xi = \xi^{(k)}_j$ does not violate the validity of our differential Schrödinger eq. (14) locally. The global matching of its solutions (15) forms the last step towards an innovated perturbation method.

### 3.2 Global solution in the $k$–th order

Under the first nontrivial choice of $N = 1$ the matching of perturbation corrections degenerates to the left asymptotic-like boundary condition at $x = L$ and its right
counterpart at $x = R$. This imposes the two linear algebraic constraints
\[
c^{(k)} C(L) + (1 - c^{(k)}) S(L) + \varepsilon \omega(L) = 0, \\
c^{(k)} C(R) + (1 - c^{(k)}) S(R) + \varepsilon \omega(R) = 0
\]
upon the energy $\varepsilon = E^{(k)}$ and coefficient $c^{(k)}(1) = 1 - d^{(k)}(1) \equiv X$,
\[
\begin{bmatrix}
S(L) - C(L), & -\omega(L) \\
S(R) - C(R), & -\omega(R)
\end{bmatrix}
\begin{bmatrix}
X \\
\varepsilon
\end{bmatrix}
= \begin{bmatrix}
S(L) \\
S(R)
\end{bmatrix}.
\]
(18)

One has to notice the possible absence of solutions of this system whenever its determinant vanishes. Such an apparent paradox just reflects an \textit{a priori} open possibility of degeneracy of the unperturbed spectrum. We only know \textit{a posteriori} that the spectrum of the one-dimensional Sturm-Liouville problem cannot degenerate at all \cite{[1]}

Let us abbreviate $c^{(k)}(j) C^{(k)}(L_i) + d^{(k)}(j) S^{(k)}(L_i) + \varepsilon \omega(L_i) + \xi_j c^{(0)}(i) = \varphi_j(L_i)$ for $N \geq 2$ and, after the next choice of $N = 2$, contemplate the four independent boundary-and-matching conditions
\[
\varphi_1(L_0) = 0, \quad \varphi_1(L_2) = \varphi_2(L_2) \quad [\equiv c^{(k)}(2) + \xi_2 c^{(0)}(2)], \\
\varphi_2(L_1) = \varphi_1(L_1) \quad [\equiv c^{(k)}(1) + \xi_1 c^{(0)}(1)], \quad \varphi_2(L_3) = 0.
\]
Both the re-normalization parameters enter these equations only in the form of their difference $Z = \xi_1 - \xi_2$. Denoting $c^{(k)}(1) = 1 - d^{(k)}(1) \equiv X$ and $c^{(k)}(2) = 1 - d^{(k)}(2) \equiv Y$ we get the four linear relations
\[
X c^{(k)}_1(L_0) + (1 - X) S^{(k)}_1(L_0) + \varepsilon \omega(L_0) = 0, \\
X c^{(k)}_1(L_2) + (1 - X) S^{(k)}_1(L_2) + \varepsilon \omega(L_2) + Z c^{(0)}(2) = Y, \\
Y c^{(k)}_2(L_1) + (1 - Y) S^{(k)}_2(L_1) + \varepsilon \omega(L_1) - Z c^{(0)}(1) = X, \\
Y c^{(k)}_2(L_3) + (1 - Y) S^{(k)}_2(L_3) + \varepsilon \omega(L_3) = 0
\]
among the four unknowns $\varepsilon$, $X$, $Y$ and $Z$. This equation is easily solved by the four-by-four matrix inversion.
At an arbitrary $N$ the general matching plus boundary formula comprises the $2N$ equations

\[
X_j C(L_j-1) + (1 - X_j) S(L_j-1) + \varepsilon \omega_j(L_j-1) = X_{j-1} + Z_j c(0)(j - 1),
\]
\[
X_j C(L_j+1) + (1 - X_j) S(L_j+1) + \varepsilon \omega_j(L_j+1) = X_{j+1} - Z_{j+1} c(0)(j + 1),
\]

where $j = 1, 2, \ldots, N$.

for $2N$ unknowns $\varepsilon$, $X_j = c(k)(j)$ and $Z_{j+1} = \xi_{j+1} - \xi_j$. Our new perturbation prescription is complete.

### 3.3 Illustration

The detailed implementation of our matching formulae is straightforward. Its best illustration is provided by the solvable square well $V^{(0)}(x) = V_{SW}(x)$ with the solvable constant perturbation $V^{(1)}(x) = \Omega$. In this extreme example the “survival of solvability” facilitates the understanding of formulae as well as a verification of their quantitative predictions without any use of a complicated algebra. For the sake of brevity we shall also pay attention to the $N = 1$ recipe in the first perturbation order only.

#### 3.3.1 Local wave functions

In the first step it is easy to extract the particular solution $\omega^{(part)}(x) = p(x) = (1/2) x \cos x$ from the non-homogeneous differential eq. (17). Its order-dependent partner eq. (16) looks similar,

\[
\left[ -\frac{d^2}{dx^2} + V^{(0)}(x) - E^{(0)} \right] C(x) = \tau(x),
\]

\[
C(x) \bigg|_{x=X} = 1, \quad \partial_x C(x) \bigg|_{x=X} = 0
\]
\[
\left[-\frac{d^2}{dx^2} + V^{(0)}(x) - E^{(0)}\right] S(x) = \tau(x),
\]

\[
S(x)\bigg|_{x=X} = 0, \quad \partial_x S(x)\bigg|_{x=X} = 1,
\]

and possesses the similar particular solution \(-\Omega p(x)\). By means of the Ansatz

\[
\omega(x) = P \sin x + Q \cos x + p(x),
\]
\[
C(x) = U \sin x + A \cos x - \Omega p(x),
\]
\[
S(x) = W \sin x + B \cos x - \Omega p(x)
\]

the initial conditions are easily satisfied by a suitable choice of the six optional constants \(P, Q, U, A, W\) and \(B\). After an elementary trigonometry using the function

\[
q(x) = \partial_x p(x) = (\cos x - x \sin x)/2
\]

and an elementary orthogonal matrix

\[
R(x) = \begin{pmatrix}
\cos x & \sin x \\
-\sin x & \cos x
\end{pmatrix} \equiv [R(-x)]^{-1}
\]

we get the result

\[
\begin{pmatrix}
P \\
Q
\end{pmatrix} = R(-X) \begin{pmatrix}
-p(X) \\
-q(X)
\end{pmatrix},
\]
\[
\begin{pmatrix}
A \\
U
\end{pmatrix} = R(-X) \begin{pmatrix}
c + \Omega p(X) \\
\Omega q(X)
\end{pmatrix}, \quad \begin{pmatrix}
B \\
W
\end{pmatrix} = R(-X) \begin{pmatrix}
\Omega p(X) \\
d + \Omega q(X)
\end{pmatrix}.
\]

Our local first-order solution is obtained by fully non-numerical means.

### 3.3.2 Global matching and the energy

Two-dimensional eq. (18) represents the physical boundary conditions at both ends of our interval of coordinates \((L, R)\). From its matrix elements

\[
\omega(L) = P, \quad \omega(R) = -(P + \pi/2), \quad C(L) = A,
\]
\[
C(R) = \Omega \pi/2 - A, \quad S(L) = B, \quad S(R) = \Omega \pi/2 - B
\]
it is easy to deduce the answer $E^{(1)} = \Omega$. This verifies the recipe and reproduces, incidentally, the exact result.

It is instructive to notice that in the traditional Rayleigh-Schrödinger approach where the value of $\varepsilon$ is evaluated in advance our boundary conditions would be satisfied automatically. In the present approach the variability of $\varepsilon$ is admitted breaking, in general, the boundary conditions

$$
\begin{bmatrix}
S(L) + \varepsilon \omega(L) & C(L) + \varepsilon \omega(L) \\
S(R) + \varepsilon \omega(R) & C(R) + \varepsilon \omega(R)
\end{bmatrix}
\begin{bmatrix}
c^{(1)} \\
d^{(1)}
\end{bmatrix} = 0.
$$

In an apparent paradox the latter equation seems quadratic (but is linear) in $\varepsilon$. Immediate calculation reveals the above-mentioned energy correction uniquely,

$$
E^{(1)} = \frac{\det\begin{bmatrix}
S(L) & C(L) \\
S(R) & C(R)
\end{bmatrix}}{
\det\begin{bmatrix}
\omega(L) & S(L) \\
\omega(R) & S(R)
\end{bmatrix} + \det\begin{bmatrix}
C(L) & \omega(L) \\
C(R) & \omega(R)
\end{bmatrix}} = \frac{\Omega \pi (B - A)/2}{\pi (B - A)/2}.
$$

Wave functions may be reproduced in the similar manner.

4 Summary

We have seen in Section 2 that for many rectangular potentials $V^{(0)}(x)$ the zero-order local wave functions are superpositions of elementary trigonometric functions $\sin \beta x$ and $\cos \beta x$ with a real or purely imaginary argument. In conclusion we should now add that for an arbitrary piece-wise polynomial perturbation this reduces the construction of corrections in perturbation series (2) to an easy algebraic exercise.
4.1 Closed formulae for polynomial perturbations

Firstly, let us notice that the inhomogeneous term \( \tau(x) \) in eq. (14) coincides with a certain superposition of products \( \langle x|k,1 \rangle = x^k \cos \beta x \) and \( \langle x|k,2 \rangle = x^k \sin \beta x \) for polynomial perturbations. These functions may be denoted and treated as a partitioned basis \( \{ |k,j \rangle \}_{j=1,2} \) with \( k = 0, 1, \ldots \). In this basis the action of the unperturbed differential operator

\[
\hat{H} = \left[ -\frac{d^2}{dx^2} + V^{(0)}(x) - E^{(0)} \right]
\]

has a closed explicit form

\[
(2\beta)^{-1}\hat{H} x \cos \beta x = \sin \beta x,
\]
\[
(4\beta^2)^{-1}\hat{H} (\beta x^2 \cos \beta x - x \sin \beta x) = x \sin \beta x,
\]
\[
(12\beta^3)^{-1}\hat{H} (2\beta^2 x^3 \cos \beta x - 3\beta x^2 \sin \beta x - 3x \cos \beta x) = x^2 \sin \beta x,
\]
\[
(8\beta^4)^{-1}\hat{H} (\beta^3 x^4 \cos \beta x - 2\beta^2 x^3 \sin \beta x - 3\beta x^2 \cos \beta x + 3x \sin \beta x) = x^3 \sin \beta x,
\]

\[
\ldots
\]

and, \textit{mutatis mutandis}, for cosines. Thus, any practical computation will immediately generalize our previous trivial constant-perturbation example.

In the constructive proof of the latter relations we firstly represent the action of our operator \( \hat{H} \) on each element of the basis as a superposition of the other basis states. It is easily shown by explicit differentiation that the coefficients of these superpositions form an infinite matrix \( Q \) with the mere three nonzero diagonals. In
the second step, we introduce a two-by-two partitioning of the matrix \( Q \) and denote

\[
Q = \begin{pmatrix}
0 & \ldots \\
b_1 & 0 & \ldots \\
c_2 & b_2 & 0 & \ldots \\
0 & c_3 & b_3 & 0 & \ldots \\
0 & 0 & c_4 & b_4 & 0 & \ldots \\
& & & & & \ddots & \ddots
\end{pmatrix}.
\]

The submatrices \( b_k = 2k\beta \sigma \) and \( c_k = -k(k-1)I \) are elementary and two-dimensional,

\[
\sigma = \sqrt{-I} = \begin{pmatrix}
0 & 1 \\
-1 & 0
\end{pmatrix}, \quad I = \begin{pmatrix}
1 & 0 \\
0 & 1
\end{pmatrix}.
\]

In the third step we verify that the left inverse \( Q^L \) of our singular matrix still exists and has the elementary form

\[
Q^L = \begin{pmatrix}
0 & b_1^{-1} & 0 & 0 & \ldots \\
0 & -b_2^{-1}c_2b_1^{-1} & b_2^{-1} & 0 & \ldots \\
0 & b_3^{-1}c_3b_2^{-1}c_2b_1^{-1} & -b_3^{-1}c_3b_2^{-1} & b_3^{-1} & \ldots \\
& & & & & \ddots & \ddots
\end{pmatrix}.
\]

The explicit form of its two-by-two submatrices remains fairly compact,

\[
(Q^L)_{nn+1} = -[2b(n+1)]^{-1}\sigma, \quad (Q^L)_{n+1n+1} = -(2b)^{-2}I
\]

\[
(Q^L)_{n+2n+1} = (2b)^{-3}(n+2)\sigma, \quad (Q^L)_{n+3n+1} = (2b)^{-4}(n+2)(n+3)I
\]

\[
(Q^L)_{n+4n+1} = -(2b)^{-5}(n+2)(n+3)(n+4)\sigma, \quad \ldots, n = 0, 1, \ldots
\]

This completes the proof. The separate rows of the non-partitioned matrix \( Q^L \) determine the particular solutions of our fundamental differential equations (16) and (17).
4.2 Generalizations

Our last observation was extremely pleasant and encouraging. It immediately implies that for the piece-wise constant unperturbed potentials our new perturbation construction remains non-numerical for each polynomial perturbation. In this sense the usual start from a harmonic oscillator may find here an unexpectedly feasible methodical alternative even in analyses of continuous models. We have seen that up to the discontinuities at the lattice points \( x = L_j, j = 1, 2, \ldots, N \) the one-dimensional or \( s \)–wave functions remained basically non-numerical.

Technical complications may emerge beyond \( s \)–waves, for polynomial \( V_j^{(0)}(x) \) and for the nonpolynomial perturbations. All these problems may appear quite naturally in many applications. In such a case both the unperturbed problem and the evaluation of corrections become much more numerical. Still, an implementation of our perturbation recipe remains virtually unchanged, consisting of the following six steps.

- **S 1.** We solve the *unperturbed* differential Schrödinger equation with the appropriate initial conditions (12) in all the domains \( J_j \). Their number \( N \) is a fixed and, presumably, very small integer parameter.

- **S 2.** We solve the linear algebraic system of the \( 2N \) *homogeneous* equations (13). This determines the unperturbed energy \( E^{(0)} \) as well as the unperturbed norms \( c_j^{(0)} \) and \( d_j^{(0)} \) of the matched zero order wave functions.

- **S 3.** We solve all the auxiliary initial-value problems (17) and generate the \( N \) functions \( \omega(x) = \omega_j(x) \). In particular, their values \( \omega_j(L_{j\pm 1}) \) have to be computed at the boundaries of all domains.
• S 4. In the given order $k = 1, 2, \ldots$ and in every domain $\mathcal{J}_j$ we specify the “input” finite sum $r_j^{(k-1)}(x)$ and solve the doublet of the initial value problems (16). This determines the functions $C_j^{(k)}(x)$ and $S_j^{(k)}(x)$ as well as their special values $C_j^{(k)}(L_j \pm 1), S_j^{(k)}(L_j \pm 1)$.

• S 5. We solve, finally, our finite set of the $2N$ “effective” or “model-space” linear algebraic eqs. (19). This defines the $k$–th energy correction $\varepsilon \equiv E^{(k)}$, the $N$ matched norms $c^{(k)}(j)$ and the $N - 1$ local re-normalization parameters $Z_j = \xi_j^{(k)} - \xi_j^{(k)}_{j-1}$ in the wave functions.

• S 6. If needed, we move to the next order $k$ and return to step S 4.

We may conclude that in the future applications of our new perturbation prescription its present algebraic (trigonometric) exemplification may be complemented by some local versions of the current semi-analytic Taylor series constructions or by the various discrete (e.g., Runge Kutta) purely numerical implementations etc.

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Figure captions

Figure 1. Momentum dependence of secular determinant (3) for four different barriers $H_1 = 10, 15, 20$ and 25.
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