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A quick perturbative method for Schrödinger equations

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Abstract. Within the framework of perturbation theory we propose, firstly, an iterative method which may serve as a source of optimal unperturbed solutions in both one and more dimensions. It combines the Runge–Kutta and Newton algorithm and its efficiency is illustrated on a few quartic oscillators. Secondly, admitting also an arbitrary perturbation of potentials we generalize the existing Runge–Kutta one-dimensional Rayleigh–Schrödinger constructions of energies and wavefunctions to more dimensions.

1. Introduction

Various applications of quantum mechanics need and use the Schrödinger equation in its standard differential form

$$-\triangle\psi(\boldsymbol{x}) + V(\boldsymbol{x})\psi(\boldsymbol{x}) = E\psi(\boldsymbol{x}). \tag{1}$$

The methods of its solution may be variational (with emphasis on the upper-bound property of the energies), perturbative (applicable simultaneously to the whole families of interactions) or purely numerical (and sufficiently quick). In the latter category, one may distinguish between the methods which are 'robust' (and converge even without any *a priori* information about the result) and the methods with a maximal efficiency (i.e. rate of convergence) [1].

The quickly convergent methods are needed, typically, whenever the solution of equation (1) must be repeated many times, say, at varying values of some parameter λ in the interaction $V(\boldsymbol{x}) = V(\lambda, \boldsymbol{x})$. In this situation, quick calculations are not always feasible: the most efficient perturbative approaches necessitate the exact solvability of equation (1) at some optimal reference value of $\lambda = \lambda_{[0]}$ [2].

Whenever all the eligible reference potentials happen to lie 'too far' [3] from the relevant (say, phenomenological) domain of parameters λ, the convergence of the perturbation series becomes prohibitively slow. At the same time, virtually all the available perturbative recipes which could eventually use an improved, unsolvable reference $V(\lambda_{[0]}, \boldsymbol{x})$ either seem prohibitively complicated [4] or employ numerical integration and take equation (1) in one dimension only [5]. In practice, as a consequence, people patiently repeat an uninspired numerical solution of the partial differential Schrödinger equation (1) as many times as required.

In the present paper, we shall circumvent the latter difficulty. Our new approach will be based on a significant improvement of the *numerical* constructions at an arbitrary dimension and initial $\lambda = \lambda_{[0]}$ (cf sections 2 and 3). In section 4 this zero-order step will be complemented by a new higher-order recipe of the *perturbative* Rayleigh–Schrödinger type for all the neighbouring $\lambda \approx \lambda_{[0]}$.

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2. Standard methods for $\lambda = \lambda_{[0]}$

2.1. One spacial dimension

Let us start our analysis from the simplest one-dimensional version

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x) + V(x)\psi(x) = E\psi(x) \tag{2}$$

of Schrödinger equation (1) with a symmetric potential $V(x) \equiv V(-x)$. It is an ordinary differential equation. At any 'trial' (i.e. not necessarily physical) energy parameter $E = E_{\mathrm{T}}$, it possesses a pair of independent solutions $\psi(x) = \psi(E, x)$ with even and odd parity. In the origin, these solutions may be normalized by the respective formulae

$$\psi(E, 0) = 1 \qquad \frac{\partial}{\partial x}\psi(E, 0) = 0 \qquad \text{parity} = \text{even} \tag{3}$$

and

$$\psi(E, 0) = 0 \qquad \frac{\partial}{\partial x}\psi(E, 0) = 1 \qquad \text{parity} = \text{odd}. \tag{4}$$

Their interpretation depends on their asymptotic behaviour. In scattering, they have to be matched to an outgoing wave at a suitable phase shift [6]. The complex energy of resonances may also be determined [7]. In the related literature the importance of a maximal computational efficiency of this matching has been emphasized many times. One may mention an unusually large number of not too dissimilar methods which compete for physicists' attention and preference [8]. In [9] the use of a thorough Padé extrapolation indicates that the careful matching is a decisive factor in an overall success of calculations.

Here, we shall only restrict ourselves to bound-state systems. The asymptotics of their wavefunctions (of both parities) remain trivial,

$$\psi(E, R) = 0 \qquad R \gg 1. \tag{5}$$

Numerically, their correct (real and discrete) energies $E = E^{(\mathrm{physical})}$ may be computed as the roots of transcendental equation (5) in the limit $R \to \infty$ [10]. The use of commercial software (e.g., MAPLE [11]) makes the practical evaluation of energies extremely comfortable.

2.2. Runge–Kutta recurrences

A recurrent code of the Runge–Kutta type may solve equation (2) at any trial energy E_{T}. With initial conditions (3) or (4), the resulting tentative wavefunction $\psi(E_{\mathrm{T}}, x)$ must pass the physical boundary-condition test (5). Otherwise, we have to search for an alternative energy candidate E'_{T}. An iterative determination of the correct $E^{(\mathrm{physical})}$ may then be based on its interval-halving localization.

Let us note that our assumption of symmetry of the potential eliminates, in effect, one of the *two* physical asymptotic conditions $\psi(E, \pm R) = 0$, $R \gg 1$. One may weaken this assumption in several ways. First, a generalization of the technique to asymmetric potentials in one dimension is immediate. For any $V(x) \neq V(-x)$ which is confining (i.e. $V(\pm\infty) > E^{(\mathrm{physical})}$) we shift the origin, $(-R, R) \longrightarrow (0, 2R)$, and employ the initialization (4).

Second, the scope of our previous considerations may be extended to central potentials $V(\boldsymbol{x}) \equiv V(x)$, $x = |\boldsymbol{x}|$ in any dimension. The related partial differential Schrödinger (1) degenerates to a sequence of its ordinary partial wave projections [6]. All of them coincide

with equation (2) with an effective potential $V^{\rm eff}(x) = \ell(\ell+1)x^{-2} + V(x)$. The acceptable, regular Runge–Kutta solutions may be normalized by the only slightly modified formula (4),

$$\psi(E, x) = x^{\ell+1} + \text{small corrections} \qquad |x| \ll 1. \tag{6}$$

One may directly return to one dimension via the choice of $\ell = -1$ (even parity) or $\ell = 0$ (odd parity). In three dimensions, integers $\ell = 0, 1, \ldots$ number the angular momenta. In K dimensions, one has only to replace ℓ by $\ell + (K-3)/2$ [12]. At large x, all these solutions share the same boundary condition (5).

A non-trivial pattern of generalization must be designed for more-dimensional forces without a central (or other) symmetry. They may describe various important phenomena (e.g., crystal surfaces in solid-state physics etc [13]). Unfortunately, even their simplest two-dimensional example is already non-trivial.

2.3. Runge–Kutta recurrences in two spacial dimensions

For simplicity, we shall only consider the non-central Schrödinger equation

$$-\frac{\partial^2}{\partial x^2}\psi(x, y) - \frac{\partial^2}{\partial y^2}\psi(x, y) + V(x, y)\psi(x, y) = E\psi(x, y) \tag{7}$$

in its most elementary Runge–Kutta discretization which replaces the kinetic energy operator $-\partial_x^2 - \partial_y^2$ by the five-term difference approximation,

$$-\frac{\partial^2}{\partial x^2}\psi(x, y) - \frac{\partial^2}{\partial y^2}\psi(x, y) = T\psi(x, y) + \mathcal{O}(h^2) \tag{8}$$

$$h^2 T\psi(x, y) = -\psi(x+h, y) - \psi(x-h, y) - \psi(x, y+h) - \psi(x, y-h) + 4\psi(x, y).$$

The obligatory transition $h \to 0$ to the exact limit will tacitly be shifted to the very end of all our subsequent considerations.

The action of T is formally defined on an infinite rectangular lattice $(x_j, y_k) = (x_0 + jh, y_0 + kh)$. A finite range of indices $j = 0, 1, \ldots, N$ and $k = 0, 1, \ldots, M+1$ specifies a relevant compact sublattice. In all the confining cases the 'edges' x_0, y_0, $x_\infty = x_0 + Nh$ and $y_\infty = y_0 + (M+1)h$ have to lie in the area where the potential is already large. This leads to the natural boundary conditions

$$\begin{aligned} &\psi(x_0, y_k) = \psi(x_N, y_k) = 0 \qquad k = 1, 2, \ldots, M \\ &\psi(x_j, y_0) = \psi(x_j, y_{M+1}) = 0 \qquad j = 0, 1, \ldots, N. \end{aligned} \tag{9}$$

An iterative selection of the true physical solutions will again be based on a tentative, partial violation of boundary conditions. In other words, we are going to treat our boundary-value Schrödinger equation via its certain initial-value re-arrangement in an arbitrary number of dimensions.

In contrast to the previous one-dimensional example, there exist many independent solutions on our planar Runge–Kutta lattice at a given energy $E_{\rm T}$. In an incomplete parallel to our one-dimensional methodical guide, let us define the nth regular solution $\psi(x_j, y_k) = \psi(n, E_{\rm T}, x_j, y_k)$ by the most trivial initialization of the left-boundary type (4),

$$\begin{aligned} &\psi(n, E_{\rm T}, x_0, y_k) = \psi(n, E_{\rm T}, x_1, y_k) = 0 \qquad k = 1, 2, \ldots, M, k \neq n \\ &\psi(n, E_{\rm T}, x_0, y_n) = 0, \psi(n, E_{\rm T}, x_1, y_n) = 1 \qquad n = 1, 2, \ldots, M. \end{aligned} \tag{10}$$

At any *fixed* grid size $h \ll 1$, our differential equation (7) becomes solvable via a separate evaluation of each of the M independent regular solutions $\psi(n, E_{\rm T}, x_j, y_k)$ in a way which

is recurrent with respect to the index j. The 'physics' represented by the full set of boundary conditions (9) will emerge only after we insert a superposition

$$\psi(E_{\rm T}, x_j, y_k) = \sum_{n=1}^{M} c_n \psi(n, E_{\rm T}, x_j, y_k) \tag{11}$$

in all boundary conditions (9) which remained unused during the Runge–Kutta recurrent evaluations themselves. We get the constraint

$$\sum_{n=1}^{M} c_n \psi(n, E_{\rm T}, x_N, y_k) = 0 \qquad k = 1, 2, \ldots, M. \tag{12}$$

Let us now simplify the notation slightly, marking M by M matrices by 'roofs' $\widehat{\ }$ and abbreviating

$$\psi(n, E_{\rm T}, x_j, y_k) \equiv (\widehat{\Psi_{\rm T}^{\{j\}}})_{k,n} \qquad k, n = 1, 2, \ldots, M. \tag{13}$$

This enables us to read equation (12) as a mere linear algebraic condition which has a non-trivial solution $\boldsymbol{c}$ if and only if its M-dimensional determinant vanishes,

$$\widehat{\Psi_{\rm T}^{\{N\}}}\boldsymbol{c} = \boldsymbol{0} \qquad \det \widehat{\Psi_{\rm T}^{\{N\}}} = 0. \tag{14}$$

Our Schrödinger equation transformed in the bidirectional Runge–Kutta recurrences $[T + V(x, y) - E_{\rm T}]\psi(E_{\rm T}, x, y) = 0$ may also be partitioned,

$$\begin{pmatrix} \widehat{W^{\{1\}}} & \hat{I} & \hat{0} & \ldots & \\ \hat{I} & \widehat{W^{\{2\}}} & \hat{I} & \hat{0} & \ldots \\ \hat{0} & \hat{I} & \widehat{W^{\{3\}}} & \hat{I} & \ldots \\ & & \ldots & \ldots & \ldots \end{pmatrix} \begin{pmatrix} \widehat{\Psi_{\rm T}^{\{1\}}} \\ \widehat{\Psi_{\rm T}^{\{2\}}} \\ \widehat{\Psi_{\rm T}^{\{3\}}} \\ \ldots \end{pmatrix} = \begin{pmatrix} \hat{0} \\ \hat{0} \\ \hat{0} \\ \ldots \end{pmatrix}. \tag{15}$$

The dynamical input information is compressed on the main diagonal,

$$(\widehat{W^{\{j\}}})_{m,n} = \begin{cases} -4 - h^2[V(x_j, y_n) - E_{\rm T}] & |m-n| = 0 \\ 1 & |m-n| = 1 \\ 0 & |m-n| > 1. \end{cases} \tag{16}$$

The initialization (10) enables us to define the regular solution in closed form, as the following determinant-like ordered products

$$\begin{aligned} \widehat{\Psi_{\rm T}^{\{1\}}} &= \hat{I} \\ \widehat{\Psi_{\rm T}^{\{2\}}} &= -\widehat{W^{\{1\}}} \\ \widehat{\Psi_{\rm T}^{\{3\}}} &= \widehat{W^{\{2\}}}\,\widehat{W^{\{1\}}} - \hat{I} \\ \widehat{\Psi_{\rm T}^{\{4\}}} &= -\widehat{W^{\{3\}}}\,\widehat{W^{\{2\}}}\,\widehat{W^{\{1\}}} + \widehat{W^{\{3\}}} + \widehat{W^{\{1\}}} \\ &\ldots. \end{aligned} \tag{17}$$

Our 'determinant of determinants' in equation (14) degenerates back to the ordinary secular determinant in one dimension [8]. *Vice versa*, at $M > 1$, the matrix equation (15) never terminates.

3. Accelerated iterations at $\lambda = \lambda_{[0]}$

If our guess E_{T} 'misses' the correct value of the energy $E^{(\mathrm{physical})}$ (and violates the physical boundary condition (5)) the differential Schrödinger equation (1) may still possess the unphysical regular solutions $\psi(E_{\mathrm{T}}, \boldsymbol{x})$. The difference $E^{(\mathrm{physical})} - E_{\mathrm{T}}$ may be treated as a product of a new energy variable $\varepsilon^{(\mathrm{physical})}$ with a 'small' (though not yet determined) auxiliary quantity δ. This induces a natural change of variables

$$E = E_{\mathrm{T}} + \delta\varepsilon \qquad \psi(E, \boldsymbol{x}) = \psi(E_{\mathrm{T}}, \boldsymbol{x}) + \delta\eta(\boldsymbol{x}) \qquad \delta \neq 0 \tag{18}$$

and transforms equation (1) into a strictly equivalent non-homogeneous equation

$$-\triangle\eta(\boldsymbol{x}) + V(\boldsymbol{x})\eta(\boldsymbol{x}) = (E_{\mathrm{T}} + \delta\varepsilon)\eta(\boldsymbol{x}) + \varepsilon\psi(E_{\mathrm{T}}, \boldsymbol{x}) \tag{19}$$

with a small parameter δ.

3.1. Newton method in one dimension

In one dimension, at a fixed old guess $E_{\mathrm{T}} \neq E^{(\mathrm{physical})}$ and at an arbitrary (i.e. physical as well as unphysical) energy shift $\delta\varepsilon$ our non-homogeneous Schrödinger equation (19) will posses a non-trivial auxiliary solution $\eta(x) = \eta(\varepsilon, E_{\mathrm{T}}, x)$ even after its trivial (i.e. much more comfortable) initialization

$$\eta(\varepsilon, E, 0) = 0 \qquad \frac{\partial}{\partial x}\eta(\varepsilon, E, 0) = 0. \tag{20}$$

After we subtract the dominant part (i.e. the original reference differential equation (2)) from our exact Schrödinger equation (19), we may omit the (single) second-order term and get the approximative differential equation

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2}\eta_{\mathrm{T}}(x) + V(x)\eta_{\mathrm{T}}(x) = E_{\mathrm{T}}\eta_{\mathrm{T}}(x) + \varepsilon_{\mathrm{T}}\psi(E_{\mathrm{T}}, x) \tag{21}$$

for corrections $\eta_{\mathrm{T}}(x) = \eta(\varepsilon_{\mathrm{T}}, E_{\mathrm{T}}, x)[1 + \mathcal{O}(\delta)]$. We encounter an apparent paradox. The latter equation has to define the new wavefunction but a variation of its argument ε_{T} may only change its norm. Indeed, it is easy to verify that

$$\eta_{\mathrm{T}}(x) = \varepsilon_{\mathrm{T}}\frac{\partial}{\partial E_{\mathrm{T}}}\psi(E_{\mathrm{T}}, x) + \mathcal{O}(\delta). \tag{22}$$

The resolution of the 'paradox' may be mediated by our auxiliary factor δ. Its variability enables us to choose a convenient norm (say, $\varepsilon_{\mathrm{T}} = 1$), to solve the pair of the initial value problems (2) + (21) and to impose the asymptotical boundary condition upon the truncated Taylor series $\psi(E, x) = \psi(E_{\mathrm{T}}, x) + \delta\eta(\varepsilon_{\mathrm{T}}, E_{\mathrm{T}}, x) + \mathcal{O}(\delta^2)$. Unexpectedly, within our first-order precision, this fixes the unique physical value of our parameter,

$$\delta = \delta_{\mathrm{T}} + \mathcal{O}(\delta_{\mathrm{T}}^2) \qquad \delta_{\mathrm{T}} = -\frac{\psi(E_{\mathrm{T}}, R)}{\eta_{\mathrm{T}}(R)} \qquad R \gg 1. \tag{23}$$

The exact energy becomes approximated in an optimal manner as well, and an extremely quick convergence of E_{T} towards its exact numerical value is achieved at an arbitrary potential,

$$\begin{aligned} &E_{\mathrm{T}} \to E'_{\mathrm{T}} \to \cdots \to E^{(\mathrm{physical})} \qquad E'_{\mathrm{T}} = E_{\mathrm{T}} + \delta_{\mathrm{T}}\varepsilon_{\mathrm{T}} \\ &E_{\mathrm{T}} - E^{(\mathrm{physical})} = \mathcal{O}(\delta) \Rightarrow E'_{\mathrm{T}} - E^{(\mathrm{physical})} = \mathcal{O}(\delta^2). \end{aligned} \tag{24}$$

Let us pick up the popular anharmonic oscillator for illustration.

3.2. Numerical test

In practical computations, the efficiency of iterations (24) will increase with the improvement of the initial $E_{\rm T}$, due to the decrease of $|\delta|$. A numerical verification of this expectation is sampled here in table 1. Our selection of the examples

$$V_{[0]}(x) = v_2 x^2 + v_4 x^4 \qquad v_4 > 0 \tag{25}$$

was inspired by the recent numerical study by Drozdov [14]. He had chosen several sets of couplings v_i in the quartic and double-well regime (i.e. with a strongly non-perturbative interpretation). By the so-called Hill-determinant method he calculated the energies with high precision. They proved useful here for comparisons (cf the last row in table 1).

Our present determination of energies uses the first derivatives (22) and is, therefore, equivalent to the Newton algorithm. Numerically, our table illustrates nicely its quadratic rate of convergence (24). After we start from a reasonably realistic guess $E_{\rm T}$, our iterations give an amazingly quickly convergent practical recipe. Our test indicates that a one-digit initial precision of $E_{\rm T}$ plus the four to six iterations already reach the ultimate limit of precision given by the ten-digit computer arithmetics of our Runge–Kutta integration.

If needed, the higher-order corrections could be introduced in the same spirit. In section 4, this will be done in full generality including also the possible changes of potentials. At the present fixed $\lambda = \lambda_{[0]}$, this would only be a straightforward exercise with limited applicability. In a self-explanatory notation, one defines the second-order corrections by the third differential equation

$$-\frac{{\rm d}^2}{{\rm d}x^2}\eta_{\rm TT}(x) + V(x)\eta_{\rm TT}(x) = E_{\rm T}\eta_{\rm TT}(x) + \varepsilon_{\rm T}\eta_{\rm T}(x) + \varepsilon_{\rm TT}\psi_{\rm T}(x) \tag{26}$$

and by the explicit second-order recipe

$$E^{(\rm physical)} = E_{\rm T} + \delta_{\rm TT}\varepsilon_T + \delta_{\rm TT}^2\varepsilon_{\rm TT} + \mathcal{O}(\delta_{\rm TT}^3) \tag{27}$$

with arbitrary norms $\varepsilon_{\rm T}$ and $\varepsilon_{\rm TT}$ and with the implicit definition

$$\psi_{\rm T}(E_{\rm T}, R) + \delta_{\rm TT}\eta_{\rm T}(\varepsilon_{\rm T}, E_{\rm T}, R) + \delta_{\rm TT}^2\eta_{\rm TT}(\varepsilon_{\rm TT}, \varepsilon_{\rm T}, E_{\rm T}, R) = 0 \tag{28}$$

of the second-order parameter $\delta_{\rm TT}$. In accord with our overall philosophy (as well as preliminary numerical tests), the smaller roots of the latter algebraic equation have to be preferred.

3.3. Newton method in more dimensions

Let us now recall equation (15), i.e. the two-dimensional partial differential Schrödinger equation at an incorrect energy $E_{\rm T}$ and in the simplest Runge–Kutta approximation of section 2. It generates the regular solutions (17) on the lattice where the sequence x_j, $j = 1, 2, \ldots, M$, means a single point in one spacial dimension and becomes a one-dimensional set in two spacial dimensions (equally well, it may be generalized to be a two-dimensional array in three spacial dimensions with $M = M' \times N'$ etc). Unfortunately, no superposition (11) can be made compatible with boundary conditions since $E_{\rm T} \neq E^{(\rm physical)}$. Changing variables (18) with $\psi(E_{\rm T}, x_j, y_k) = (\widehat{\Psi_{\rm T}^{\{j\}}}\boldsymbol{c}_{\rm T})_k$, we may only write down the discretized Schrödinger equation (19),

$$[T + V(x, y) - E_{\rm T}]\eta(\varepsilon, E_{\rm T}, x, y) = \varepsilon\psi(E_{\rm T}, x, y) + \delta\varepsilon\eta(\varepsilon, E_{\rm T}, x, y) \tag{29}$$

and omit the negligible corrections. Under the assumption

$$\eta(\varepsilon_{\rm T}, E_{\rm T}, x_j, y_k) = \eta_{\rm T}(x_j, y_k)[1 + \mathcal{O}(\delta)] \qquad \eta_{\rm T}(x_j, y_k) = \widehat{\Phi^{\{j\}}}\boldsymbol{c}_{\rm T} \qquad \widehat{\Phi^{\{1\}}} = \hat{0} \tag{30}$$

Table 1. The quartic-oscillator energies after J iterations in the ten-digit arithmetics of MAPLE (last column: [14]).

			J						
v_2	v_4	R	0	1	2	3	4	5	∞
−1.000	0.0025	8.0	−8.5	−8.639	−8.6131	−8.611 883 2	−8.611 880 720	−8.611 880 720	−8.611 880 719
−1.000	0.0025	9.0	−8.5	−8.640	−8.6132	−8.611 884 0	−8.611 880 721	−8.611 880 721	−8.611 880 719
−1.000	0.0025	9.0	−6.0	−5.953	−5.949 752	−5.949 734 588	−5.949 734 587	−5.949 734 587	−5.949 734 590
0.000	1.0000	3.0	1.0	1.0588	1.060 3610	1.060 362 12	1.060 362 12	1.060 362 12	1.060 362 09
−2.000	1.0000	3.0	0.14	0.137 7856	0.137 788 29	0.137 788 29	0.137 788 29	0.137 788 29	—

this leads to the replacement of our original Schrödinger equation by the coupled pair of Runge–Kutta recurrences

$$(T+V-E_{\rm T})\widehat{\Psi_{\rm T}^{\{j\}}}=\hat{0}\qquad (T+V-E_{\rm T})\widehat{\Phi_{\rm T}^{\{j\}}}=\varepsilon_{\rm T}\widehat{\Psi_{\rm T}^{\{j\}}}\qquad j=1,2,\ldots,N. \tag{31}$$

Finally, after the same trivial choice of the norm $\varepsilon_{\rm T}=1$ as above, the boundary conditions acquire the linear homogeneous form

$$(\widehat{\Psi_{\rm T}^{\{N\}}}+\delta\widehat{\Phi_{\rm T}^{\{N\}}}+\mathcal{O}(\delta^2))\boldsymbol{c}_{\rm T}=\mathbf{0}. \tag{32}$$

Within the error bounds $\mathcal{O}(\delta_{\rm T}^2)$ it defines the coefficients $\boldsymbol{c}_{\rm T}$. The necessary condition (of vanishing of the *linearized* secular determinant) also gives the explicit $\delta_{\rm T}$. It depends on M and generalizes the ratio (23) to more spacial dimensions.

4. Perturbation corrections near $\lambda_{[0]}$

4.1. Rayleigh–Schrödinger series

The methods of our preceding text provide a (numerical) knowledge of a bound-state wavefunction $\psi_{[0]}(\boldsymbol{x})$ and its energy $E_{[0]}$ at a fixed potential $V(\lambda_{[0]},\boldsymbol{x})\equiv V_{[0]}(\boldsymbol{x})$. Now, we intend to solve the whole set of Schrödinger equations (1) with potentials

$$V(\lambda,\boldsymbol{x})=V_{[0]}(\boldsymbol{x})+(\lambda-\lambda_{[0]})V_{[1]}(\boldsymbol{x})+(\lambda-\lambda_{[0]})^2V_{[2]}(\boldsymbol{x})+\cdots. \tag{33}$$

For this purpose, we shall use the Rayleigh–Schrödinger perturbation ansatz

$$\psi(\boldsymbol{x})=\psi_{[0]}(\boldsymbol{x})+(\lambda-\lambda_{[0]})\psi_{[1]}(\boldsymbol{x})+(\lambda-\lambda_{[0]})^2\psi_{[2]}(\boldsymbol{x})+\cdots \tag{34}$$

$$E=E_{[0]}+(\lambda-\lambda_{[0]})E_{[1]}+(\lambda-\lambda_{[0]})^2E_{[2]}+\cdots. \tag{35}$$

In any number of dimensions this splits our differential Schrödinger equation (1) into its $\lambda\to\lambda_{[0]}$ zero-order version

$$(H_{[0]}-E_{[0]})\psi_{[0]}(\boldsymbol{x})=0 \tag{36}$$

accompanied by the hierarchy of the (in more than one dimension, partial) differential equations for corrections,

$$\begin{aligned}(H_{[0]}-E_{[0]})\psi_{[1]}(\boldsymbol{x})&=-H_{[1]}\psi_{[0]}(\boldsymbol{x})+E_{[1]}\psi_{[0]}(\boldsymbol{x})\\ (H_{[0]}-E_{[0]})\psi_{[2]}(\boldsymbol{x})&=-H_{[2]}\psi_{[0]}(\boldsymbol{x})-(H_{[1]}-E_{[1]})\psi_{[1]}(\boldsymbol{x})+E_{[2]}\psi_{[0]}(\boldsymbol{x})\ldots.\end{aligned} \tag{37}$$

In a compact notation, all these equations possess the same non-homogeneous form

$$(H_{[0]}-E_{[0]})\psi_{[k]}(\boldsymbol{x})=\tau_{[k-1]}(\boldsymbol{x})+E_{[k]}\psi_{[0]}(\boldsymbol{x}) \tag{38}$$

with the obvious abbreviation $\tau_{[k-1]}(\boldsymbol{x})$ for 'known' terms. These equations should define corrections $E_{[k]}$ and $\psi_{[k]}(\boldsymbol{x})$ in terms of their predecessors (we may easily infer that $\tau_{[0]}(\boldsymbol{x})=H_{[1]}\psi_{[0]}(\boldsymbol{x})$ etc).

4.2. The ansatz of Skála and Čížek

We may note a close practical complementarity of our 'non-standard' zero-order recipe of section 3.1 with the recent developments of the Rayleigh–Schrödinger perturbation theory in one spacial dimension as offered by Skála and Čížek [5] and further developed in [15–18]. A common idea of all these prescriptions may be found in a combined use of Runge–Kutta recurrences and boundary conditions. In particular, in [5, 15] the evaluation of the first- and higher-order Rayleigh–Schrödinger corrections has implicitly been based on some known

(typically, harmonic oscillator) zero-order input while the authors of [16, 18] have noted that it is sufficient to evaluate this input by the standard numerical methods.

The most important theoretical step towards the feasibility of construction of expansions (34) and (35) around *arbitrary* $\lambda_{[0]}$ has been made in [5] where the (*a priori*, arbitrary) dependence of $\psi_{[k]}(\boldsymbol{x})$ on the *variable* energy $E_{[k]}$ has been fixed as linear. After a thorough further study of this conjecture [15] it became clear that the proper ansatz should rather be two-parametrical,

$$\psi_{[k]}(\boldsymbol{x}) = \varphi_{[k]}(\boldsymbol{x}) + E_{[k]}\chi_{[k]}(\boldsymbol{x}) + F\psi_{[0]}(\boldsymbol{x}) \tag{39}$$

keeping trace of the (obvious) renormalization ambiguity of $\psi_{[k]}(\boldsymbol{x})$. The second variable $F = F_{[k]}(E_{[k]})$ may influence the Runge–Kutta recurrences and its role will be discussed later; the variability of $E_{[k]}$ in equation (39) gives

$$[T_{[0]} + V_{[0]}(\boldsymbol{x}) - E_{[0]}]\varphi_{[k]}(\boldsymbol{x}) = \tau_{[k-1]}(\boldsymbol{x}) \tag{40}$$

$$[T_{[0]} + V_{[0]}(\boldsymbol{x}) - E_{[0]}]\chi(\boldsymbol{x}) = \psi_{[0]}(\boldsymbol{x}) \tag{41}$$

i.e. in effect it splits equation (38) in two parts.

4.3. More than one dimension

The most important practical condition of applicability of the whole perturbative recipe in one spacial dimension lies in a quick numerical solvability of the zero-order equation (36). Hence the effort of the preceding two sections. Still, as we have already mentioned, the importance of our accelerated evaluation of $E_{[0]}$ further increases, significantly, after a transition to the more spacial dimensions. Unfortunately, in this generalization, the appropriate Rayleigh–Schrödinger formalism has not yet been published in any explicit detail.

For completeness, we are going to fill this gap here. Our reason lies not only in an enhancement of importance of our iterative method of section 3.3 (by showing a new and broad area of its applicability in future computations) but also in an immanent challenging mathematics. Indeed, in spite of an existing overall belief in a feasibility of calculations with the ansatz (39) and equations (40) and (41) in more dimensions [17], only a few incomplete studies are known to us which have paid attention to the related technicalities [19].

Let us now return to two spacial dimensions. The partial differential equation (38) with kernel

$$H_{[0]} - E_{[0]} \equiv -\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + V(\lambda_{[0]}, x, y) - E_{[0]} \tag{42}$$

is not invertible and a re-normalization $\psi_{[k]}(x, y) +$ constant $\times\, \psi_{[0]}(x, y)$ of its solutions is permitted. In a way which extends the one-dimensional pseudo-inversion construction [5, 16] we may discretize the two-dimensional equations (40) and (41), i.e. in the notation of section 2.3 write

$$[T + V(\lambda_{[0]}, x, y) - E_{[0]}]\varphi_{[k]}(x, y) = \tau_{[k-1]}(x, y) \qquad \varphi_{[k]}(x_j, y_m) = (\widehat{\mathcal{A}^{\{j\}}}\boldsymbol{a})_m \tag{43}$$

$$[T + V(\lambda_{[0]}, x, y) - E_{[0]}]\chi_{[k]}(x, y) = \psi_{[0]}(x, y) \qquad \chi_{[k]}(x_j, y_m) = (\widehat{\mathcal{B}^{\{j\}}}\boldsymbol{b})_m \tag{44}$$

with some auxiliary (though not yet fully specified) analogues $\widehat{\mathcal{A}^{\{j\}}}$ and $\widehat{\mathcal{B}^{\{j\}}}$ of our above Runge–Kutta regular solution matrices $\widehat{\Psi_{\mathrm{T}}^{\{j\}}}$ and $\widehat{\Phi_{\mathrm{T}}^{\{j\}}}$, respectively.

4.4. The choice of normalization

Having dropped the leading-order subscripts $[k]$ with $k > 0$ as redundant, we may start from equation (40) and re-write it in a transparent and recurrent Runge–Kutta form

$$\begin{pmatrix} \hat{I} & \hat{0} & \dots & & \hat{0} \\ \widehat{W^{\{2\}}} & \hat{I} & \hat{0} & \dots & \hat{0} \\ \hat{I} & \widehat{W^{\{3\}}} & \hat{I} & \hat{0} & \dots \\ \hat{0} & \ddots & \ddots & \ddots & \hat{0} \\ \hat{0} & \dots & \hat{I} & \widehat{W^{\{N-1\}}} & \hat{I} \end{pmatrix} \begin{pmatrix} \widehat{\mathcal{A}^{\{2\}}}\boldsymbol{a} \\ \widehat{\mathcal{A}^{\{3\}}}\boldsymbol{a} \\ \widehat{\mathcal{A}^{\{4\}}}\boldsymbol{a} \\ \dots \\ \widehat{\mathcal{A}^{\{N\}}}\boldsymbol{a} \end{pmatrix} = \begin{pmatrix} \boldsymbol{\tau}_{[k-1]}^{\{1\}} - \widehat{W^{\{1\}}}\widehat{\mathcal{A}^{\{1\}}}\boldsymbol{a} \\ \boldsymbol{\tau}_{[k-1]}^{\{2\}} - \widehat{\mathcal{A}^{\{1\}}}\boldsymbol{a} \\ \boldsymbol{\tau}_{[k-1]}^{\{3\}} \\ \dots \\ \boldsymbol{\tau}_{[k-1]}^{\{N-1\}} \end{pmatrix}. \tag{45}$$

Now, the second parameter F enters the game—we shall employ its variability and postulate

$$\sum_{m=1}^{M} a_m = 1 \qquad \widehat{\mathcal{A}^{\{1\}}} = \hat{I}. \tag{46}$$

This enables us to glue the M identical columns $\boldsymbol{\tau}_{[k-1]}^{\{j\}}$ into a matrix $\widehat{\tau^{\{j\}}}$ and to get rid of vectors $\boldsymbol{a}$ in equation (45) completely,

$$\begin{pmatrix} \hat{I} & \hat{0} & \dots & & & \hat{0} \\ \widehat{W^{\{2\}}} & \hat{I} & \hat{0} & \dots & & \hat{0} \\ \hat{I} & \widehat{W^{\{3\}}} & \hat{I} & \hat{0} & \dots & \hat{0} \\ \hat{0} & \ddots & \ddots & \ddots & & \hat{0} \\ \hat{0} & \ddots & \hat{I} & \widehat{W^{\{N-2\}}} & \hat{I} & \hat{0} \\ \hat{0} & \dots & \hat{0} & \hat{I} & \widehat{W^{\{N-1\}}} & \hat{I} \end{pmatrix} \begin{pmatrix} \widehat{\mathcal{A}^{\{2\}}} \\ \widehat{\mathcal{A}^{\{3\}}} \\ \widehat{\mathcal{A}^{\{4\}}} \\ \widehat{\mathcal{A}^{\{5\}}} \\ \dots \\ \widehat{\mathcal{A}^{\{N\}}} \end{pmatrix} = \begin{pmatrix} \widehat{\tau^{\{1\}}} - \widehat{W^{\{1\}}} \\ \widehat{\tau^{\{2\}}} - \hat{I} \\ \widehat{\tau^{\{3\}}} \\ \widehat{\tau^{\{4\}}} \\ \vdots \\ \widehat{\tau^{\{N-1\}}} \end{pmatrix}. \tag{47}$$

This is an equation which defines all the matrices $\widehat{\mathcal{A}^{\{j\}}}$ step by step.

Mutatis mutandis, analogous manipulations have to be applied to equation (44) for functions χ. In a way inspired by equation (30) we shall use the simplest $\hat{\mathcal{B}}^{\{1\}} = \hat{0}$. One of the first consequences is obtained when we contemplate the ansatz (39) at $x = x_1$, $\boldsymbol{c} = \boldsymbol{a} + E_{[k]}\widehat{\mathcal{B}^{\{1\}}}\boldsymbol{b} + F(E_{[k]})\boldsymbol{c}_{[0]}$. No ambiguity is left—it defines the unique renormalization

$$F = \frac{\sum_{m=1}^{M}(\boldsymbol{c}_{[k]})_m - 1}{\sum_{m=1}^{M}(\boldsymbol{c}_{[0]})_m}. \tag{48}$$

4.5. Boundary conditions

The order independence of $\chi_{[k]}(x, y) = \chi_{[0]}(x, y)$ is accompanied by the degenerate form of the M-dimensional matrices $\hat{\mathcal{B}}^{\{j\}}$ (composed of the M identical columns $\boldsymbol{\mathcal{B}}^{\{j\}}$ due to the trivial initialization $\hat{\mathcal{B}}^{\{1\}} = \hat{0}$). As a consequence, we obtain the simpler, vectorial form of the related Runge–Kutta recurrences which implicitly define $\hat{\mathcal{B}}^{\{j\}}$,

$$\begin{pmatrix} \hat{I} & \hat{0} & \dots & & & \hat{0} \\ \widehat{W^{\{2\}}} & \hat{I} & \hat{0} & \dots & & \hat{0} \\ \hat{I} & \widehat{W^{\{3\}}} & \hat{I} & \hat{0} & \dots & \hat{0} \\ \hat{0} & \ddots & \ddots & \ddots & & \hat{0} \\ \hat{0} & \ddots & \hat{I} & \widehat{W^{\{N-2\}}} & \hat{I} & \hat{0} \\ \hat{0} & \dots & \hat{0} & \hat{I} & \widehat{W^{\{N-1\}}} & \hat{I} \end{pmatrix} \begin{pmatrix} \mathcal{B}^{\{2\}} \\ \mathcal{B}^{\{3\}} \\ \mathcal{B}^{\{4\}} \\ \vdots \\ \mathcal{B}^{\{N-1\}} \\ \mathcal{B}^{\{N\}} \end{pmatrix} = \begin{pmatrix} \boldsymbol{\psi}_{[0]}^{\{1\}} \\ \boldsymbol{\psi}_{[0]}^{\{2\}} \\ \boldsymbol{\psi}_{[0]}^{\{3\}} \\ \ddots \\ \boldsymbol{\psi}_{[0]}^{\{N-2\}} \\ \boldsymbol{\psi}_{[0]}^{\{N-1\}} \end{pmatrix}. \tag{49}$$

All these components of χ result from the inversion of the same triangular matrix as above. We could call the inverse of this matrix (shared by both equations) an unperturbed propagator. After all, one could 'glue' equations (43) and (44) together and add the vector $\boldsymbol{\mathcal{B}}$ as an additional row to the matrix $\hat{\mathcal{A}}$ itself.

In a way generalizing the one-dimensional constructions, the formula for energies will follow from the asymptotic boundary condition applied to our kth-order wavefunction. For lattices with $M > 1$, the determination of the parameter $E_{[k]}$ becomes coupled to the determination of the M superposition coefficients a_m constrained by the (re)normalization condition (46). In such an arrangement we get the asymptotics

$$\widehat{\mathcal{A}^{\{N\}}}_{[k]}\boldsymbol{a}_{[k]} + \boldsymbol{\mathcal{B}}^{\{N\}}E_{[k]} = \mathbf{0} \tag{50}$$

coupled to equation (46). This makes the final equation non-homogeneous,

$$\begin{pmatrix} \mathcal{A}^{\{N\}}_{11} & \mathcal{A}^{\{N\}}_{12} & \dots & \mathcal{A}^{\{N\}}_{1M} & \mathcal{B}^{\{N\}}_{1} \\ \mathcal{A}^{\{N\}}_{21} & \mathcal{A}^{\{N\}}_{22} & \dots & \mathcal{A}^{\{N\}}_{2M} & \mathcal{B}^{\{N\}}_{2} \\ & & \dots & & \\ \mathcal{A}^{\{N\}}_{M1} & \mathcal{A}^{\{N\}}_{M2} & \dots & \mathcal{A}^{\{N\}}_{MM} & \mathcal{B}^{\{N\}}_{M} \\ 1 & 1 & \dots & 1 & 0 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_M \\ E_{[k]} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}. \tag{51}$$

By the routine matrix inversion, these $M + 1$ *linear* equations define the M unknown coefficients $(a_{[k]})_j$, $j = 1, 2, \dots, M$ *and* the energy $E_{[k]}$. Up to the exceptional singular cases (which are not excluded but may be regularized, for example, by a change of the grid length h), this leads to the explicit form of energies (and, simultaneously, wavefunctions) given by Cramer's rule in each perturbation order.

5. Summary

We have described a new approach to the family of Schrödinger equations (1) at some set of couplings (or other parameters) λ in the potential. We have assumed that all these parameters λ lie in a small vicinity of some reference value $\lambda_{[0]}$ which *does not* make the unperturbed potential solvable.

Our new proposal consists of two methodically entirely independent parts. The first is purely numerical and is restricted to the single reference interaction only at an arbitrary fixed $\lambda_{[0]}$. In this zero-order context, the routine trial and error fit of the recurrent (here, Runge–Kutta) solutions to physical asymptotics is recalled. In a search for eigenvalues we recommend the Newton iterative approach. This is a drastic recipe which, in effect, uses several recurrent Runge–Kutta constructions per single iteration. At such a cost we eliminate any need for the universal accelerators of convergence [20].

Numerically, this was demonstrated in a test restricted, for simplicity, to one spacial dimension. The expected quick (namely, quadratic) rate of convergence of iterations has been verified on a few double wells. Its performance encouraged us to generalize our bound-state implementation of Newton iterations to more dimensions.

The second part of our proposal is a new perturbative method. We shared its main inspiration with the recent one-dimensional proposal by Fernández and Guardiola [18] (the text of which had only become known to us after the submission but before revision of this paper) relying upon the common recurrent spirit of both perturbation theory and numerical (viz, Runge–Kutta) discretized constructions.

In spite of an initial optimism [17], the original variable-energy idea (as applied in one dimension by Skála and Čížek [5]) did not suffice for an easy transition to more dimensions [15]. Fortunately, by accepting the more general matrix-propagator point of view of [4, 19] and by using, in effect, as many as M other auxiliary variables (with $M \to \infty$ in principle) we were able to overcome the methodical barrier and to extend the Runge–Kutta perturbative method to more than one dimension in a fairly universal manner.

The second, perturbative half of our text seems optimally tailored for correcting the iterative zero-order numerical solutions of its first half. In the future, both these halves might find a common area of applicability as a mixed, 'numerically-perturbative' method. Due to their common recurrent background, a full power of their combination might emerge in analyses of families of potentials with a variable coupling λ and in an *absence of simplification* of the Schrödinger equation(s) near *any* particular value $\lambda_{[0]}$.

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