Renormalized Numerov method for multi-channel system

Duy Tan University, Danang, Vietnam
Kazuhito Mizuyama

April 13, 2026

Chapter 1

Renormalized Numerov method for multi-channel system

1.1 Numerov method for multi-channel system

In this section, we describe the multichannel version of the Numerov method. The Numerov method is a specialized numerical technique for solving second-order linear differential equations that lack a first-derivative term, typically of the form $y''(x) = f(x)y(x) + g(x)$. Originally introduced by B. V. Numerov for celestial mechanics [1, 2], the method achieves a high local truncation error of $\mathcal{O}(h^6)$ (global error of $\mathcal{O}(h^4)$) while requiring only one evaluation of the potential per step. This efficiency and accuracy make it particularly well-suited for solving the Schrödinger equation in quantum mechanics [3].

Let us consider the channel coupled differential equation is given by

$$\left[\frac{\partial^2}{\partial r^2}\mathbf{1} + \boldsymbol{V}(r)\right]\vec{\phi}(r) = 0 \tag{1.1}$$

where $\mathbf{1}$ is the N-dimensional unit matrix, $\boldsymbol{V}(r)$ is the symmetric $N \times N$-matrix potential and $\vec{\phi}(r)$ is the N-dimensional vector.

Eq.(1.1) can be solved by the Numerov method. Using the Numerov method, Eq.(1.1) can be solved by calculating the following recurrence relation:

$$\boldsymbol{A}(r_{n+1})\vec{\phi}(r_{n+1}) - \boldsymbol{B}(r_n)\vec{\phi}(r_n) + \boldsymbol{A}(r_{n-1})\vec{\phi}(r_{n-1}) = \mathcal{O}(h^6), \tag{1.2}$$

where

$$\boldsymbol{A}(r_n) = \mathbf{1} + \frac{1}{12}h^2\boldsymbol{V}(r_n) \tag{1.3}$$

$$\boldsymbol{B}(r_n) = 2\left(\mathbf{1} - \frac{5}{12}h^2\boldsymbol{V}(r_n)\right) \tag{1.4}$$

Note that $\boldsymbol{A}$ and $\boldsymbol{B}$ are also $N \times N$ matrices.

A system of $N \times N$ second-order differential equations has N distinct solution vectors, obtained by imposing N different boundary conditions. Therefore, using these N solution vectors, we can define an $N \times N$ solution matrix $\mathbf{\Phi}$ as

$$\mathbf{\Phi} \equiv \begin{pmatrix} \vec{\phi}^{(1)} & \vec{\phi}^{(2)} & \cdots & \vec{\phi}^{(N)} \end{pmatrix} \tag{1.5}$$

This solution matrix satisfies

$$\left[\frac{\partial^2}{\partial r^2}\mathbf{1} + \boldsymbol{V}(r)\right]\mathbf{\Phi}(r) = 0 \tag{1.6}$$

and the recursive formula of the Numerov method for the solution matrix is given by

$$\boldsymbol{A}(r_{n+1})\mathbf{\Phi}(r_{n+1}) - \boldsymbol{B}(r_n)\mathbf{\Phi}(r_n) + \boldsymbol{A}(r_{n-1})\mathbf{\Phi}(r_{n-1}) = \boldsymbol{\mathcal{O}}(h^6), \tag{1.7}$$

1.2 Renormalized Numerov method

The renormalized Numerov method was developed to overcome the numerical instabilities inherent in the standard Numerov method, particularly when dealing with classically forbidden regions or closed channels where solutions can grow or decay exponentially [4]. Instead of propagating the wave functions directly, this method propagates the ratio of the solution matrices at adjacent steps, known as the ratio matrix. This approach effectively suppresses numerical divergence and maintains the linear independence of solutions while preserving the high $\mathcal{O}(h^4)$ accuracy of the original Numerov algorithm. It shares a conceptual foundation with the log-derivative method [5] but integrates it into the high-precision framework of the Numerov scheme.

By introducing

$$\boldsymbol{F}(r_n) \equiv \boldsymbol{A}(r_n)\boldsymbol{\Phi}(r_n) \tag{1.8}$$

$$\boldsymbol{U}(r_n) \equiv \boldsymbol{B}(r_n)\boldsymbol{A}^{-1}(r_n) \tag{1.9}$$

Eq.(1.7) can be rewritten as

$$\boldsymbol{F}(r_{n+1}) - \boldsymbol{U}(r_n)\boldsymbol{F}(r_n) + \boldsymbol{F}(r_{n-1}) = \boldsymbol{\mathcal{O}}(h^6) \tag{1.10}$$

1.2.1 For regular solution

When $\boldsymbol{F}(r_n)$ is defined using regular solutions $\boldsymbol{\Phi}^{(r)}(r_n)$, i.e.

$$\boldsymbol{F}^{(r)}(r_n) \equiv \boldsymbol{A}(r_n)\boldsymbol{\Phi}^{(r)}(r_n) \tag{1.11}$$

let the ratio matrix $\boldsymbol{M}^{(r)}(r_n)$ be defined as

$$\boldsymbol{M}^{(r)}(r_n) \equiv \boldsymbol{F}^{(r)}(r_n)\boldsymbol{F}^{(r)-1}(r_{n-1}) \tag{1.12}$$

Eq.(1.10) becomes as

$$\boldsymbol{M}^{(r)}(r_{n+1}) - \boldsymbol{U}(r_n) + \boldsymbol{M}^{(r)-1}(r_n) = \boldsymbol{\mathcal{O}}(h^6) \tag{1.13}$$

Assuming that $\boldsymbol{F}^{(r)}(r_0)$ and $\boldsymbol{F}^{(r)}(r_1)$ are given as initial conditions, and since $\boldsymbol{F}^{(r)}(r_0) = 0$ is often specified for regular solutions, we have $\boldsymbol{M}^{(r)-1}(r_1) = 0$. Therefore Eq.(1.13) can be solved recursively as

$$\boldsymbol{M}^{(r)}(r_2) = \boldsymbol{U}(r_1) \tag{1.14}$$

$$\boldsymbol{M}^{(r)}(r_3) = \boldsymbol{U}(r_2) - \boldsymbol{M}^{(r)-1}(r_2) \tag{1.15}$$

$$\vdots$$

$$\boldsymbol{M}^{(r)}(r_N) = \boldsymbol{U}(r_{N-1}) - \boldsymbol{M}^{(r)-1}(r_{N-1}) \tag{1.16}$$

Using $\boldsymbol{M}(r_2), \cdots, \boldsymbol{M}(r_N)$ obtained in this way, $\boldsymbol{F}^{(r)}(r_2), \cdots, \boldsymbol{F}^{(r)}(r_N)$ can be calculated as

$$\boldsymbol{F}^{(r)}(r_2) = \boldsymbol{M}^{(r)}(r_2)\boldsymbol{F}^{(r)}(r_1) \tag{1.17}$$

$$\boldsymbol{F}^{(r)}(r_3) = \boldsymbol{M}^{(r)}(r_3)\boldsymbol{F}^{(r)}(r_2) \tag{1.18}$$

$$\vdots$$

$$\boldsymbol{F}^{(r)}(r_N) = \boldsymbol{M}^{(r)}(r_N)\boldsymbol{F}^{(r)}(r_{N-1}). \tag{1.19}$$

according to its definition (1.12).

Finally, the solution matrix can be obtained as follows.

$$\boldsymbol{\Phi}^{(r)}(r_1) = \boldsymbol{A}^{-1}(r_1)\boldsymbol{F}^{(r)}(r_1) \tag{1.20}$$

$$\boldsymbol{\Phi}^{(r)}(r_2) = \boldsymbol{A}^{-1}(r_2)\boldsymbol{F}^{(r)}(r_2) \tag{1.21}$$

$$\vdots$$

$$\boldsymbol{\Phi}^{(r)}(r_N) = \boldsymbol{A}^{-1}(r_N)\boldsymbol{F}^{(r)}(r_N). \tag{1.22}$$

1.2.2 For irregular solution

When $\boldsymbol{F}(r_n)$ is defined using irregular solutions $\boldsymbol{\Phi}^{(\pm)}(r_n)$, i.e.

$$\boldsymbol{F}^{(\pm)}(r_n) \equiv \boldsymbol{A}(r_n)\boldsymbol{\Phi}^{(\pm)}(r_n) \tag{1.23}$$

let the ratio matrix $\boldsymbol{M}^{(\pm)}(r_n)$ be defined as

$$\boldsymbol{M}^{(\pm)}(r_n) \equiv \boldsymbol{F}^{(\pm)}(r_{n-1})\boldsymbol{F}^{(\pm)-1}(r_n) \tag{1.24}$$

Eq.(1.10) becomes as

$$\boldsymbol{M}^{(\pm)-1}(r_{n+1}) - \boldsymbol{U}(r_n) + \boldsymbol{M}^{(\pm)}(r_n) = \mathcal{O}(h^6). \tag{1.25}$$

Assuming that $\boldsymbol{F}^{(\pm)}(r_N)$ and $\boldsymbol{F}^{(\pm)}(r_{N-1})$ are given as boundary conditions, we have

$$\boldsymbol{M}^{(\pm)}(r_N) \equiv \boldsymbol{F}^{(\pm)}(r_{N-1})\boldsymbol{F}^{(\pm)-1}(r_N) \tag{1.26}$$

and Eq.(1.25) can be solved recursively as

$$\boldsymbol{M}^{(\pm)}(r_{N-1}) = \boldsymbol{U}(r_{N-1}) - \boldsymbol{M}^{(\pm)-1}(r_N) \tag{1.27}$$

$$\boldsymbol{M}^{(\pm)}(r_{N-2}) = \boldsymbol{U}(r_{N-2}) - \boldsymbol{M}^{(\pm)-1}(r_{N-1}) \tag{1.28}$$

$$\vdots$$

$$\boldsymbol{M}^{(\pm)}(r_1) = \boldsymbol{U}(r_1) - \boldsymbol{M}^{(\pm)-1}(r_2) \tag{1.29}$$

$\boldsymbol{F}^{(\pm)}(r_1), \cdots, \boldsymbol{F}^{(\pm)}(r_{N-2})$ can be calculated as

$$\boldsymbol{F}^{(\pm)}(r_{N-2}) = \boldsymbol{M}^{(\pm)}(r_{N-1})\boldsymbol{F}^{(\pm)}(r_{N-1}) \tag{1.30}$$

$$\vdots$$

$$\boldsymbol{F}^{(\pm)}(r_1) = \boldsymbol{M}^{(\pm)}(r_2)\boldsymbol{F}^{(\pm)}(r_2) \tag{1.31}$$

according to its definition (1.24).

Finally, the solution matrix can be obtained as follows.

$$\boldsymbol{\Phi}^{(\pm)}(r_1) = \boldsymbol{A}^{-1}(r_1)\boldsymbol{F}^{(\pm)}(r_1) \tag{1.32}$$

$$\boldsymbol{\Phi}^{(\pm)}(r_2) = \boldsymbol{A}^{-1}(r_2)\boldsymbol{F}^{(\pm)}(r_2) \tag{1.33}$$

$$\vdots$$

$$\boldsymbol{\Phi}^{(\pm)}(r_N) = \boldsymbol{A}^{-1}(r_N)\boldsymbol{F}^{(\pm)}(r_N). \tag{1.34}$$

1.3 Wronskian

The Wronskian between the regular and irregular solutions of the system given by Eq.(1.1) is given by

$$\boldsymbol{W}\left(\boldsymbol{\Phi}^{(r)}, \boldsymbol{\Phi}^{(\pm)}\right) = \boldsymbol{\Phi}^{(r)\mathsf{T}}\frac{\partial \boldsymbol{\Phi}^{(\pm)}}{\partial r} - \frac{\partial \boldsymbol{\Phi}^{(r)\mathsf{T}}}{\partial r}\boldsymbol{\Phi}^{(\pm)}. \tag{1.35}$$

It can be proven by Green's theorem that the Wronskian, defined in this way, is independent of coordinates when $\boldsymbol{V}$ is symmetric in Eq.(1.1). Within the framework of renormalised Numerov, it is possible to obtain a high-precision, coordinate-independent finite-difference representation of the Wronskian.

We evaluate $\boldsymbol{W}$ at the midpoint $r = (r_n + r_{n-1})/2$. Let $h = r_n - r_{n-1}$. The Taylor expansions of $\boldsymbol{\Phi}_n \equiv \boldsymbol{\Phi}(r + h/2)$ and $\boldsymbol{\Phi}_{n-1} \equiv \boldsymbol{\Phi}(r - h/2)$ around the midpoint r are:

$$\boldsymbol{\Phi}_n = \boldsymbol{\Phi}(r) + \frac{h}{2}\frac{\partial \boldsymbol{\Phi}(r)}{\partial r} + \frac{h^2}{8}\frac{\partial^2 \boldsymbol{\Phi}(r)}{\partial r^2} + \frac{h^3}{48}\frac{\partial^3 \boldsymbol{\Phi}(r)}{\partial r^3} + \mathcal{O}(h^4), \tag{1.36}$$

$$\boldsymbol{\Phi}_{n-1} = \boldsymbol{\Phi}(r) - \frac{h}{2}\frac{\partial \boldsymbol{\Phi}(r)}{\partial r} + \frac{h^2}{8}\frac{\partial^2 \boldsymbol{\Phi}(r)}{\partial r^2} - \frac{h^3}{48}\frac{\partial^3 \boldsymbol{\Phi}(r)}{\partial r^3} + \mathcal{O}(h^4). \tag{1.37}$$

From the sum and difference of these expansions, we have the following midpoint expressions:

$$\boldsymbol{\Phi}(r) = \frac{\boldsymbol{\Phi}_n + \boldsymbol{\Phi}_{n-1}}{2} - \frac{h^2}{8}\frac{\partial^2 \boldsymbol{\Phi}}{\partial r^2} + \mathcal{O}(h^4), \tag{1.38}$$

$$\frac{\partial \boldsymbol{\Phi}(r)}{\partial r} = \frac{\boldsymbol{\Phi}_n - \boldsymbol{\Phi}_{n-1}}{h} - \frac{h^2}{24}\frac{\partial^3 \boldsymbol{\Phi}(r)}{\partial r^3} + \mathcal{O}(h^4). \tag{1.39}$$

Using $\frac{\partial^2 \boldsymbol{\Phi}(r)}{\partial r^2} = -\boldsymbol{V}\boldsymbol{\Phi}(r)$ and $\frac{\partial^3 \boldsymbol{\Phi}(r)}{\partial r^3} = -\frac{\partial(\boldsymbol{V}\boldsymbol{\Phi}(r))}{\partial r}$ from Eq. (1.1):

$$\boldsymbol{\Phi}(r) = \frac{\boldsymbol{\Phi}_n + \boldsymbol{\Phi}_{n-1}}{2} + \frac{h^2}{8}\boldsymbol{V}\boldsymbol{\Phi}(r) + \mathcal{O}(h^4), \tag{1.40}$$

$$\frac{\partial \boldsymbol{\Phi}(r)}{\partial r} = \frac{\boldsymbol{\Phi}_n - \boldsymbol{\Phi}_{n-1}}{h} + \frac{h^2}{24}\frac{\partial(\boldsymbol{V}\boldsymbol{\Phi}(r))}{\partial r} + \mathcal{O}(h^4). \tag{1.41}$$

Substituting these into Eq. (1.35):

$$\begin{aligned}\boldsymbol{W} &= \left[\frac{\boldsymbol{\Phi}_n^{(r)} + \boldsymbol{\Phi}_{n-1}^{(r)}}{2} + \frac{h^2}{8}\boldsymbol{V}\boldsymbol{\Phi}^{(r)}\right]^{\mathsf{T}} \left[\frac{\boldsymbol{\Phi}_n^{(\pm)} - \boldsymbol{\Phi}_{n-1}^{(\pm)}}{h} + \frac{h^2}{24}(\boldsymbol{V}\boldsymbol{\Phi}^{(\pm)})'\right] \\ &- \left[\frac{\boldsymbol{\Phi}_n^{(r)} - \boldsymbol{\Phi}_{n-1}^{(r)}}{h} + \frac{h^2}{24}(\boldsymbol{V}\boldsymbol{\Phi}^{(r)})'\right]^{\mathsf{T}} \left[\frac{\boldsymbol{\Phi}_n^{(\pm)} + \boldsymbol{\Phi}_{n-1}^{(\pm)}}{2} + \frac{h^2}{8}\boldsymbol{V}\boldsymbol{\Phi}^{(\pm)}\right] + \mathcal{O}(h^4).\end{aligned} \tag{1.42}$$

Thus, the continuous Wronskian at the midpoint is:

$$\boldsymbol{W} = \frac{\boldsymbol{\Phi}_{n-1}^{(r)\mathsf{T}}\boldsymbol{\Phi}_n^{(\pm)} - \boldsymbol{\Phi}_n^{(r)\mathsf{T}}\boldsymbol{\Phi}_{n-1}^{(\pm)}}{h} + \frac{h^2}{6}[\boldsymbol{\Phi}^{(r)\mathsf{T}}\boldsymbol{V}\boldsymbol{\Phi}^{(\pm)\prime} - \boldsymbol{\Phi}^{(r)\prime\mathsf{T}}\boldsymbol{V}\boldsymbol{\Phi}^{(\pm)}] + \mathcal{O}(h^4). \tag{1.43}$$

Applying the following identity to the second term,

$$\boldsymbol{\Phi}^{(r)\mathsf{T}}\boldsymbol{V}\boldsymbol{\Phi}^{(\pm)\prime} - \boldsymbol{\Phi}^{(r)\prime\mathsf{T}}\boldsymbol{V}\boldsymbol{\Phi}^{(\pm)} = \frac{\boldsymbol{\Phi}_{n-1}^{(r)\mathsf{T}}\boldsymbol{V}\boldsymbol{\Phi}_n^{(\pm)} - \boldsymbol{\Phi}_n^{(r)\mathsf{T}}\boldsymbol{V}\boldsymbol{\Phi}_{n-1}^{(\pm)}}{h} + \mathcal{O}(h^2). \tag{1.44}$$

we obtain $\boldsymbol{W}$ as

$$\boldsymbol{W} = \frac{1}{h}\left[\boldsymbol{\Phi}_{n-1}^{(r)\mathsf{T}}\left(\mathbf{1} + \frac{h^2}{6}\boldsymbol{V}\right)\boldsymbol{\Phi}_n^{(\pm)} - \boldsymbol{\Phi}_n^{(r)\mathsf{T}}\left(\mathbf{1} + \frac{h^2}{6}\boldsymbol{V}\right)\boldsymbol{\Phi}_{n-1}^{(\pm)}\right] + \mathcal{O}(h^4). \tag{1.45}$$

Eq.(1.44) can be easily proven by substituting the first two terms of the right-hand side of Eqs.(1.36) and (1.37) into $\boldsymbol{\Phi}_n$ and $\boldsymbol{\Phi}_{n-1}$ on the right-hand side of Eq.(1.44) as follows:

$$\begin{aligned}&\frac{\boldsymbol{\Phi}_{n-1}^{(r)\mathsf{T}}\boldsymbol{V}\boldsymbol{\Phi}_n^{(\pm)} - \boldsymbol{\Phi}_n^{(r)\mathsf{T}}\boldsymbol{V}\boldsymbol{\Phi}_{n-1}^{(\pm)}}{h} \\ &= \frac{1}{h}\left[\left(\boldsymbol{\Phi}^{(r)} - \frac{h}{2}\boldsymbol{\Phi}^{(r)\prime}\right)^{\mathsf{T}}\boldsymbol{V}\left(\boldsymbol{\Phi}^{(\pm)} + \frac{h}{2}\boldsymbol{\Phi}^{(\pm)\prime}\right) - \left(\boldsymbol{\Phi}^{(r)} + \frac{h}{2}\boldsymbol{\Phi}^{(r)\prime}\right)^{\mathsf{T}}\boldsymbol{V}\left(\boldsymbol{\Phi}^{(\pm)} - \frac{h}{2}\boldsymbol{\Phi}^{(\pm)\prime}\right)\right] + \mathcal{O}(h^2) \\ &= \frac{1}{h}\left[\left(\boldsymbol{\Phi}^{(r)\mathsf{T}}\boldsymbol{V}\boldsymbol{\Phi}^{(\pm)} + \frac{h}{2}\boldsymbol{\Phi}^{(r)\mathsf{T}}\boldsymbol{V}\boldsymbol{\Phi}^{(\pm)\prime} - \frac{h}{2}\boldsymbol{\Phi}^{(r)\prime\mathsf{T}}\boldsymbol{V}\boldsymbol{\Phi}^{(\pm)} - \frac{h^2}{4}\boldsymbol{\Phi}^{(r)\prime\mathsf{T}}\boldsymbol{V}\boldsymbol{\Phi}^{(\pm)\prime}\right)\right. \\ &\left. - \left(\boldsymbol{\Phi}^{(r)\mathsf{T}}\boldsymbol{V}\boldsymbol{\Phi}^{(\pm)} - \frac{h}{2}\boldsymbol{\Phi}^{(r)\mathsf{T}}\boldsymbol{V}\boldsymbol{\Phi}^{(\pm)\prime} + \frac{h}{2}\boldsymbol{\Phi}^{(r)\prime\mathsf{T}}\boldsymbol{V}\boldsymbol{\Phi}^{(\pm)} - \frac{h^2}{4}\boldsymbol{\Phi}^{(r)\prime\mathsf{T}}\boldsymbol{V}\boldsymbol{\Phi}^{(\pm)\prime}\right)\right] + \mathcal{O}(h^2) \\ &= \boldsymbol{\Phi}^{(r)\mathsf{T}}\boldsymbol{V}\boldsymbol{\Phi}^{(\pm)\prime} - \boldsymbol{\Phi}^{(r)\prime\mathsf{T}}\boldsymbol{V}\boldsymbol{\Phi}^{(\pm)} + \mathcal{O}(h^2)\end{aligned} \tag{1.46}$$

Although Eq.(1.44) is a second-order approximation, substituting it into the second term of Eq.(1.43) results in a fourth-order approximation for that term, and Eq.(1.43) as a whole thus becomes a fourth-order approximation.

Finally, we relate the matrix $\mathbf{1} + \frac{h^2}{6}\boldsymbol{V}$ to the product of Numerov factors $\boldsymbol{A}_n = \mathbf{1} + \frac{h^2}{12}\boldsymbol{V}_n$:

$$\boldsymbol{A}_{n-1}\boldsymbol{A}_n = \left(\mathbf{1} + \frac{h^2}{12}\boldsymbol{V}_{n-1}\right)\left(\mathbf{1} + \frac{h^2}{12}\boldsymbol{V}_n\right) = \mathbf{1} + \frac{h^2}{12}(\boldsymbol{V}_{n-1} + \boldsymbol{V}_n) + \mathcal{O}(h^4) = \mathbf{1} + \frac{h^2}{6}\boldsymbol{V}(r) + \mathcal{O}(h^4). \tag{1.47}$$

Substituting Eq. (1.47) into Eq. (1.45) and using $\boldsymbol{A}_n^{\mathsf{T}} = \boldsymbol{A}_n$:

$$\boldsymbol{W} = \frac{(\boldsymbol{A}_{n-1}\boldsymbol{\Phi}_{n-1}^{(r)})^{\mathsf{T}}(\boldsymbol{A}_n\boldsymbol{\Phi}_n^{(\pm)}) - (\boldsymbol{A}_n\boldsymbol{\Phi}_n^{(r)})^{\mathsf{T}}(\boldsymbol{A}_{n-1}\boldsymbol{\Phi}_{n-1}^{(\pm)})}{h} + \mathcal{O}(h^4). \tag{1.48}$$

Equation (1.48) leads naturally to the definition of the renormalized variables $\boldsymbol{F}_n \equiv \boldsymbol{A}_n\boldsymbol{\Phi}_n$, yielding the final discrete form $\boldsymbol{W}_n$:

$$\boldsymbol{W} = \frac{\boldsymbol{F}_{n-1}^{(r)\mathsf{T}}\boldsymbol{F}_n^{(\pm)} - \boldsymbol{F}_n^{(r)\mathsf{T}}\boldsymbol{F}_{n-1}^{(\pm)}}{h} \equiv \boldsymbol{W}_n. \tag{1.49}$$

1.3.1 Proof of exact coordinate independence

We prove that $\boldsymbol{W}_n$ is strictly constant for any n. From the Numerov recurrence $\boldsymbol{F}_{n+1} = \boldsymbol{U}_n\boldsymbol{F}_n - \boldsymbol{F}_{n-1}$ where $\boldsymbol{U}_n = \boldsymbol{B}_n\boldsymbol{A}_n^{-1}$ is symmetric:

$$\begin{aligned} h\boldsymbol{W}_{n+1} &= \boldsymbol{F}_n^{(r)\mathsf{T}}\boldsymbol{F}_{n+1}^{(\pm)} - \boldsymbol{F}_{n+1}^{(r)\mathsf{T}}\boldsymbol{F}_n^{(\pm)} \\ &= \boldsymbol{F}_n^{(r)\mathsf{T}}(\boldsymbol{U}_n\boldsymbol{F}_n^{(\pm)} - \boldsymbol{F}_{n-1}^{(\pm)}) - (\boldsymbol{U}_n\boldsymbol{F}_n^{(r)} - \boldsymbol{F}_{n-1}^{(r)})^{\mathsf{T}}\boldsymbol{F}_n^{(\pm)} \\ &= \boldsymbol{F}_n^{(r)\mathsf{T}}\boldsymbol{U}_n\boldsymbol{F}_n^{(\pm)} - \boldsymbol{F}_n^{(r)\mathsf{T}}\boldsymbol{F}_{n-1}^{(\pm)} - \boldsymbol{F}_n^{(r)\mathsf{T}}\boldsymbol{U}_n^{\mathsf{T}}\boldsymbol{F}_n^{(\pm)} + \boldsymbol{F}_{n-1}^{(r)\mathsf{T}}\boldsymbol{F}_n^{(\pm)} \\ &= \boldsymbol{F}_{n-1}^{(r)\mathsf{T}}\boldsymbol{F}_n^{(\pm)} - \boldsymbol{F}_n^{(r)\mathsf{T}}\boldsymbol{F}_{n-1}^{(\pm)} = h\boldsymbol{W}_n. \end{aligned} \tag{1.50}$$

Thus, $\boldsymbol{W}_{n+1} = \boldsymbol{W}_n$ holds exactly, providing strict coordinate independence.

Bibliography

[1] B. V. Numerov, “A method of extrapolation of perturbations”, *Monthly Notices of the Royal Astronomical Society*, Vol. 84, pp. 592–601 (1924).

[2] B. V. Numerov, “Note on the numerical integration of $d^2x/dt^2 = f(x,t)$”, *Astronomische Nachrichten*, Vol. 230, pp. 359–364 (1927).

[3] J. M. Blatt, “Practical points on numerical integration of the Schrödinger equation”, *Journal of Computational Physics*, Vol. 1, pp. 382–396 (1967).

[4] B. R. Johnson, “New numerical methods for solving the Schrödinger equation”, *The Journal of Chemical Physics*, Vol. 67, pp. 4086–4091 (1977).

[5] B. R. Johnson, “The multichannel log-derivative method for scattering calculations”, *Journal of Computational Physics*, Vol. 13, pp. 445–449 (1973).