Numerical algorithms

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I. NUMEROV METHOD

The Taylor expansion of the function $\phi(x)$ up to 5th order is defined by

$$\begin{aligned}\phi(x) &= \phi(x_0) + (x-x_0)\,\frac{\partial\phi(x)}{\partial x}\bigg|_{x=x_0} + \frac{1}{2}(x-x_0)^2\,\frac{\partial^2\phi(x)}{\partial x^2}\bigg|_{x=x_0}\\ &+\frac{1}{3!}(x-x_0)^3\,\frac{\partial^3\phi(x)}{\partial x^3}\bigg|_{x=x_0} + \frac{1}{4!}(x-x_0)^4\,\frac{\partial^4\phi(x)}{\partial x^4}\bigg|_{x=x_0} + \frac{1}{5!}(x-x_0)^5\,\frac{\partial^5\phi(x)}{\partial x^5}\bigg|_{x=x_0} + \mathcal{O}(h^6) \qquad (1)\end{aligned}$$

If we define

$$\phi_n \equiv \phi(x_n) \qquad (2)$$
$$\phi_{n+1} \equiv \phi(x_n+h) \qquad (3)$$
$$\phi_{n-1} \equiv \phi(x_n-h) \qquad (4)$$

then we obtain

$$\phi_{n+1} = \phi_n + h\,\frac{\partial\phi(x)}{\partial x}\bigg|_n + \frac{1}{2}h^2\,\frac{\partial^2\phi(x)}{\partial x^2}\bigg|_n + \frac{1}{3!}h^3\,\frac{\partial^3\phi(x)}{\partial x^3}\bigg|_n + \frac{1}{4!}h^4\,\frac{\partial^4\phi(x)}{\partial x^4}\bigg|_n + \frac{1}{5!}h^5\,\frac{\partial^5\phi(x)}{\partial x^5}\bigg|_n + \mathcal{O}(h^6) \qquad (5)$$
$$\phi_{n-1} = \phi_n - h\,\frac{\partial\phi(x)}{\partial x}\bigg|_n + \frac{1}{2}h^2\,\frac{\partial^2\phi(x)}{\partial x^2}\bigg|_n - \frac{1}{3!}h^3\,\frac{\partial^3\phi(x)}{\partial x^3}\bigg|_n + \frac{1}{4!}h^4\,\frac{\partial^4\phi(x)}{\partial x^4}\bigg|_n - \frac{1}{5!}h^5\,\frac{\partial^5\phi(x)}{\partial x^5}\bigg|_n + \mathcal{O}(h^6) \qquad (6)$$

The sum of (5) and (6) gives

$$\phi_{n+1}+\phi_{n-1} = 2\phi_n + h^2\,\frac{\partial^2\phi(x)}{\partial x^2}\bigg|_n + \frac{1}{12}h^4\,\frac{\partial^4\phi(x)}{\partial x^4}\bigg|_n + \mathcal{O}(h^6) \qquad (7)$$

Now if we suppose $\phi(x)$ satisfies the differential equation,

$$\left[\frac{\partial^2}{\partial x^2} + V(x)\right]\phi(x) = 0 \qquad (8)$$

Then (7) becomes

$$\phi_{n+1}+\phi_{n-1} = 2\phi_n - h^2 V(x_n)\phi_n + \frac{1}{12}h^4\,\frac{\partial^4\phi(x)}{\partial x^4}\bigg|_n + \mathcal{O}(h^6) \qquad (9)$$

On the other hand, from (8), we can obtain

$$\begin{aligned}\frac{\partial^4\phi(x)}{\partial x^4} &= -\frac{\partial^2}{\partial x^2}\left[V(x)\phi(x)\right]\\ &\sim -\frac{1}{h^2}\left[V(x_{n+1})\phi_{n+1} - 2V(x_n)\phi_n + V(x_{n-1})\phi_{n-1}\right] + \mathcal{O}(h^2) \qquad (10)\end{aligned}$$

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By inserting (10) into (9), we obtain

$$\phi_{n+1} + \phi_{n-1} \;=\; 2\phi_n - h^2 V(x_n)\phi_n - \frac{1}{12}h^2\left[V(x_{n+1})\phi_{n+1} - 2V(x_n)\phi_n + V(x_{n-1})\phi_{n-1}\right] + \mathcal{O}(h^6) \tag{11}$$

Finally we obtain

$$\left(1 + \frac{1}{12}h^2 V(x_{n+1})\right)\phi_{n+1} - 2\left(1 - \frac{5}{12}h^2 V(x_n)\right)\phi_n + \left(1 + \frac{1}{12}h^2 V(x_{n-1})\right)\phi_{n-1} = \mathcal{O}(h^6) \tag{12}$$

If we set

$$A_n \;\equiv\; 1 + \frac{1}{12}h^2 V(x_n) \tag{13}$$

$$B_n \;\equiv\; 2\left(1 - \frac{5}{12}h^2 V(x_n)\right) \tag{14}$$

Eq.(12) becomes as

$$A_{n+1}\phi_{n+1} - B_n\phi_n + A_{n-1}\phi_{n-1} = \mathcal{O}(h^6). \tag{15}$$

Suppose the mesh points are given as $n \in (0, 1, 2, \cdots, N)$, and ϕ_0 and ϕ_1 is given as the initial condition; then Eq.(15) can be solved as

$$\phi_2 \;=\; \frac{1}{A_2}\left(B_1\phi_1 - A_0\phi_0\right) \tag{16}$$

$$\phi_3 \;=\; \frac{1}{A_3}\left(B_2\phi_2 - A_1\phi_1\right) \tag{17}$$

$$\vdots$$

$$\phi_N \;=\; \frac{1}{A_N}\left(B_{N-1}\phi_{N-1} - A_{N-2}\phi_{N-2}\right) \tag{18}$$

If we solve the equation from the outside, we can solve using the boundary conditions ϕ_N and ϕ_{N-1} as

$$\phi_{N-2} \;=\; \frac{1}{A_{N-2}}\left(B_{N-1}\phi_{N-1} - A_N\phi_N\right) \tag{19}$$

$$\phi_{N-3} \;=\; \frac{1}{A_{N-3}}\left(B_{N-2}\phi_{N-2} - A_{N-1}\phi_{N-1}\right) \tag{20}$$

$$\vdots$$

$$\phi_1 \;=\; \frac{1}{A_1}\left(B_2\phi_2 - A_3\phi_3\right) \tag{21}$$

A. Numerical derivative

The difference of (5) and (6) gives

$$\phi_{n+1} - \phi_{n-1} \;=\; 2h\left.\frac{\partial\phi(x)}{\partial x}\right|_n + \frac{1}{3}h^3\left.\frac{\partial^3\phi(x)}{\partial x^3}\right|_n + \mathcal{O}(h^5) \tag{22}$$

On the other hand, from (8), we can obtain

$$\left.\frac{\partial^3\phi(x)}{\partial x^3}\right|_n \;=\; -\left.\frac{\partial}{\partial x}\left[V(x)\phi(x)\right]\right|_n$$

$$\sim\; -\frac{1}{2h}\left[V(x_{n+1})\phi_{n+1} - V(x_{n-1})\phi_{n-1}\right] + \mathcal{O}(h^2) \qquad \text{[3-point formula(32)]} \tag{23}$$

By inserting (23) into (22), we obtain

$$\left.\frac{\partial\phi(x)}{\partial x}\right|_n \;=\; \frac{1}{2h}\left[\left(1 + \frac{1}{6}h^2 V(x_{n+1})\right)\phi_{n+1} - \left(1 + \frac{1}{6}h^2 V(x_{n-1})\right)\phi_{n-1}\right] + \mathcal{O}(h^5) \tag{24}$$

Note that this is better approximation than the 5-point formula (41).

II. THE LAGRANGE POLYNOMIAL METHOD

According to the Lagrange polynomial, the function $\phi(x)$ can be described by

$$\phi(x) \sim \sum_{k=0}^{n} \phi(x_k) L_k(x) \tag{25}$$

where

$$L_k(x) = \prod_{m(\neq k),0\leq m\leq n} \frac{x - x_m}{x_k - x_m} \tag{26}$$

By using this Lagrange polynomial, it is well known that n-point numerical derivative formula is given by

$$f'(x_j) \sim \sum_{k=0}^{n} \phi(x_k) L'_k(x_j) + \mathcal{O}(h^{n-1}) \tag{27}$$

where

$$L'_k(x_j) = \left.\frac{\partial L_k(x)}{\partial x}\right|_{x=x_j} \tag{28}$$

A. 3-points formula

We set 3-points as

$$\phi_n \equiv \phi(x_n) \tag{29}$$

$$\phi_{n+1} \equiv \phi(x_n + h) \tag{30}$$

$$\phi_{n-1} \equiv \phi(x_n - h) \tag{31}$$

Then we can obtain the numerical derivative formula by using (27),

$$f'(x_n) \sim \phi_{n-1} L'_{n-1}(x_n) + \phi_n L'_n(x_n) + \phi_{n+1} L'_{n+1}(x_n) + \mathcal{O}(h^2) = \frac{\phi_{n+1} - \phi_{n-1}}{2h} + \mathcal{O}(h^2) \tag{32}$$

where

$$L_{n-1}(x) = \frac{x - x_n}{x_{n-1} - x_n} \frac{x - x_{n+1}}{x_{n-1} - x_{n+1}} = \frac{1}{2h^2}(x - x_n)(x - x_{n+1}) \to L'_{n-1}(x_n) = -\frac{1}{2h} \tag{33}$$

$$L_n(x) = \frac{x - x_{n-1}}{x_n - x_{n-1}} \frac{x - x_{n+1}}{x_n - x_{n+1}} = -\frac{1}{h^2}(x - x_{n-1})(x - x_{n+1}) \to L'_n(x_n) = 0 \tag{34}$$

$$L_{n+1}(x) = \frac{x - x_{n-1}}{x_{n+1} - x_{n-1}} \frac{x - x_n}{x_{n+1} - x_n} = \frac{1}{2h^2}(x - x_{n-1})(x - x_n) \to L'_{n+1}(x_n) = \frac{1}{2h} \tag{35}$$

B. 5-points formula

We set 5-points as

$$\phi_n \equiv \phi(x_n) \tag{36}$$

$$\phi_{n+1} \equiv \phi(x_n + h) \tag{37}$$

$$\phi_{n-1} \equiv \phi(x_n - h) \tag{38}$$

$$\phi_{n+2} \equiv \phi(x_n + 2h) \tag{39}$$

$$\phi_{n-2} \equiv \phi(x_n - 2h) \tag{40}$$

Then we can obtain the numerical derivative formula by using (27),

$$\begin{aligned} f'(x_n) &\sim \phi_{n-2} L'_{n-2}(x_n) + \phi_{n-1} L'_{n-1}(x_n) + \phi_n L'_n(x_n) + \phi_{n+1} L'_{n+1}(x_n) + \phi_{n+2} L'_{n+2}(x_n) + \mathcal{O}(h^4) \\ &= \frac{1}{12h}\left(-\phi_{n+2} + 8\phi_{n+1} - 8\phi_{n-1} + \phi_{n-2}\right) + \mathcal{O}(h^4) \end{aligned} \tag{41}$$

where

$$
\begin{aligned}
L_{n-2}(x) &= \frac{1}{24h^4}(x-x_{n-1})(x-x_n)(x-x_{n+1})(x-x_{n+2}) \to L'_{n-2}(x_n) = \frac{1}{12h} && (42)\\
L_{n-1}(x) &= -\frac{1}{6h^4}(x-x_{n-2})(x-x_n)(x-x_{n+1})(x-x_{n+2}) \to L'_{n-1}(x_n) = -\frac{2}{3h} && (43)\\
L_{n}(x) &= \frac{1}{4h^4}(x-x_{n-2})(x-x_{n-1})(x-x_{n+1})(x-x_{n+2}) \to L'_{n}(x_n) = 0 && (44)\\
L_{n+1}(x) &= -\frac{1}{6h^4}(x-x_{n-2})(x-x_{n-1})(x-x_n)(x-x_{n+2}) \to L'_{n+1}(x_n) = \frac{2}{3h} && (45)\\
L_{n+2}(x) &= \frac{1}{24h^4}(x-x_{n-2})(x-x_{n-1})(x-x_n)(x-x_{n+2}) \to L'_{n+2}(x_n) = -\frac{1}{12h} && (46)
\end{aligned}
$$

III. STURM-LIOUVILLE EQUATION AND NUMEROV METHOD.

The Sturm-Liouville equation takes the form,

$$\left[\frac{\partial}{\partial r}M(r)\frac{\partial}{\partial r} + U(r)\right]\phi(r) = \lambda\phi(r) \tag{47}$$

With this equation, if we suppose $u(r)$ which is the regular solution at the origin and $v(r)$ is the solution satisfies the out-going boundary condition respectively. The Wronskian W is defined by using $u(r)$ and $v(r)$,

$$W \equiv M(r)\left(u(r)\frac{\partial v(r)}{\partial r} - v(r)\frac{\partial u(r)}{\partial r}\right) \tag{48}$$

The derivative of the Wronskian is

$$
\begin{aligned}
\frac{\partial W}{\partial r} &= \frac{\partial}{\partial r}\left[M(r)\left(u(r)\frac{\partial v(r)}{\partial r} - v(r)\frac{\partial u(r)}{\partial r}\right)\right]\\
&= \frac{\partial M(r)}{\partial r}\left(u(r)\frac{\partial v(r)}{\partial r} - v(r)\frac{\partial u(r)}{\partial r}\right) + M(r)\left(u(r)\frac{\partial^2 v(r)}{\partial r^2} - v(r)\frac{\partial^2 u(r)}{\partial r^2}\right)\\
&= u(r)\frac{\partial M(r)}{\partial r}\frac{\partial v(r)}{\partial r} + u(r)M(r)\frac{\partial^2 v(r)}{\partial r^2} - v(r)\frac{\partial M(r)}{\partial r}\frac{\partial u(r)}{\partial r} - v(r)M(r)\frac{\partial^2 u(r)}{\partial r^2}\\
&= u(r)\frac{\partial}{\partial r}M(r)\frac{\partial}{\partial r}v(r) - v(r)\frac{\partial}{\partial r}M(r)\frac{\partial}{\partial r}u(r) = u(r)\left(\lambda - U(r)\right)v(r) - v(r)\left(\lambda - U(r)\right)u(r) = 0 && (49)
\end{aligned}
$$

Therefore $W = const$ for r.

If we transform the wave function as $\phi(r) = M^{-\frac{1}{2}}(r)\psi(r)$,

$$
\begin{aligned}
\frac{\partial}{\partial r}M(r)\frac{\partial}{\partial r}\phi(r) &= \frac{\partial}{\partial r}M(r)\frac{\partial}{\partial r}M^{-\frac{1}{2}}(r)\psi(r)\\
&= M^{\frac{1}{2}}(r)\frac{\partial^2\psi(r)}{\partial r^2} + \frac{1}{4}M^{-\frac{1}{2}}(r)\left[\frac{1}{M(r)}\left(\frac{\partial M(r)}{\partial r}\right)^2 - 2\frac{\partial^2 M(r)}{\partial r^2}\right]\psi(r) && (50)
\end{aligned}
$$

therefore (47) can be written by

$$\left[\frac{\partial^2}{\partial r^2} + \tilde{U}(r)\right]\psi(r) = \frac{\lambda}{M(r)}\psi(r) \tag{51}$$

where

$$\tilde{U}(r) = \frac{U(r)}{M(r)} + \frac{1}{4M(r)}\left[\frac{1}{M(r)}\left(\frac{\partial M(r)}{\partial r}\right)^2 - 2\frac{\partial^2 M(r)}{\partial r^2}\right] \tag{52}$$

By replacing $u(r) = M^{-\frac{1}{2}}(r)\psi(r)$ and $v(r) = M^{-\frac{1}{2}}(r)g(r)$, the Wronskian becomes

$$W \equiv M(r)\left(u(r)\frac{\partial v(r)}{\partial r} - v(r)\frac{\partial u(r)}{\partial r}\right)$$

$$= M(r)\left(u(r)\frac{\partial}{\partial r}M^{-\frac{1}{2}}(r)g(r) - v(r)\frac{\partial}{\partial r}M^{-\frac{1}{2}}(r)\psi(r)\right)$$

$$= M(r)\left(M^{-\frac{1}{2}}(r)\psi(r)\frac{\partial}{\partial r}M^{-\frac{1}{2}}(r)g(r) - M^{-\frac{1}{2}}(r)g(r)\frac{\partial}{\partial r}M^{-\frac{1}{2}}(r)\psi(r)\right)$$

$$= \left(\psi(r)\frac{\partial}{\partial r}g(r) - g(r)\frac{\partial}{\partial r}\psi(r)\right) \tag{53}$$

IV. FINITE-DIFFERENCE REPRESENTATIONS OF THE WRONSKIAN

Let the equation to be solved be given as

$$\left[\frac{\partial^2}{\partial x^2} + V(x)\right]\phi(x) = 0 \tag{54}$$

let the regular and irregular solutions be denoted by u and $v^{(+)}$, respectively, and let their Wronskian be defined as

$$W(u, v^{(+)}) \equiv u(x)\frac{\partial v^{(+)}(x)}{\partial x} - \frac{\partial u(x)}{\partial x}v^{(+)}(x). \tag{55}$$

It is well known that, although the Wronskian is define as a function of the coordinate x, it is a quantity that does not depend on the coordinate. However, even when performing numerical calculations as defined, coordinate dependence does not disappear entirely.

We shall therefore derive a finite difference formula for the Wronskian that guarantees the absence of coordinate dependence. In order to derive a finite difference representation of the Wronskian that is independent of coordinates, we evaluate the Wronskian at a point x, which is the midpoint between x_n and x_{n-1} (i.e. $x = (x_n + x_{n-1})/2$).

The Taylor expansions of $\phi_n(= \phi(x_n))$ and $\phi_{n-1}(= \phi(x_{n-1}))$ around x are given by

$$\phi_n = \phi(x) + \frac{h}{2}\phi'(x) + \frac{1}{2}\left(\frac{h}{2}\right)^2\phi''(x) + \frac{1}{3!}\left(\frac{h}{2}\right)^3\phi'''(x) + \frac{1}{4!}\left(\frac{h}{2}\right)^4\phi^{(4)}(x) + \mathcal{O}(h^5) \tag{56}$$

$$\phi_{n-1} = \phi(x) - \frac{h}{2}\phi'(x) + \frac{1}{2}\left(\frac{h}{2}\right)^2\phi''(x) - \frac{1}{3!}\left(\frac{h}{2}\right)^3\phi'''(x) + \frac{1}{4!}\left(\frac{h}{2}\right)^4\phi^{(4)}(x) + \mathcal{O}(h^5) \tag{57}$$

respectively, by using Eq.(1) with

$$x_n - x = \frac{x_n - x_{n-1}}{2} = \frac{h}{2}. \tag{58}$$

Therefore we can obtain

$$\phi_n - \phi_{n-1} = h\phi'(x) + \frac{h^3}{24}\phi'''(x) + \mathcal{O}(h^5) \tag{59}$$

$$\phi_n + \phi_{n-1} = 2\phi(x) + \frac{h^2}{4}\phi''(x) + \mathcal{O}(h^4) \tag{60}$$

Since $\phi'''(x) = -\frac{\partial}{\partial x}(V(x)\phi(x))$ and $\phi''(x) = -V(x)\phi(x)$ due to Eq.(54), Eqs.(59) and (60) can be rewritten as

$$\phi_n - \phi_{n-1} = h\phi'(x) - \frac{h^3}{24}\frac{\partial}{\partial x}(V(x)\phi(x)) + \mathcal{O}(h^5) \tag{61}$$

$$\phi_n + \phi_{n-1} = 2\phi(x) - \frac{h^2}{4}V(x)\phi(x) + \mathcal{O}(h^4). \tag{62}$$

Therefore we obtain

$$\phi'(x) = \frac{\phi_n - \phi_{n-1}}{h} + \frac{h^2}{24}\frac{\partial}{\partial x}(V(x)\phi(x)) + \mathcal{O}(h^4) \tag{63}$$

$$\phi(x) = \frac{\phi_n + \phi_{n-1}}{2} + \frac{h^2}{8}V(x)\phi(x) + \mathcal{O}(h^4). \tag{64}$$

Applying Eqs.(63) and (64) to the r.h.s of Eq.(55), we obtain

$$
\begin{aligned}
W(u,v^{(+)}) &= u(x)\frac{\partial v^{(+)}(x)}{\partial x} - \frac{\partial u(x)}{\partial x}v^{(+)}(x) \\
&= \left(\frac{u_n+u_{n-1}}{2} + \frac{h^2}{8}V(x)u(x)\right)\left(\frac{v_n^{(+)}-v_{n-1}^{(+)}}{h} + \frac{h^2}{24}\frac{\partial}{\partial x}\left(V(x)v^{(+)}(x)\right)\right) \\
&\quad - \left(\frac{u_n-u_{n-1}}{h} + \frac{h^2}{24}\frac{\partial}{\partial x}\left(V(x)u(x)\right)\right)\left(\frac{v_n^{(+)}+v_{n-1}^{(+)}}{2} + \frac{h^2}{8}V(x)v^{(+)}(x)\right) + \mathcal{O}(h^4). \qquad (65) \\
&= \left(\frac{u_n+u_{n-1}}{2}\right)\left(\frac{v_n^{(+)}-v_{n-1}^{(+)}}{h}\right) - \left(\frac{u_n-u_{n-1}}{h}\right)\left(\frac{v_n^{(+)}+v_{n-1}^{(+)}}{2}\right) \\
&\quad + \left(\frac{u_n+u_{n-1}}{2}\right)\frac{h^2}{24}\frac{\partial}{\partial x}\left(V(x)v^{(+)}(x)\right) + \frac{h^2}{8}V(x)u(x)\left(\frac{v_n^{(+)}-v_{n-1}^{(+)}}{h}\right) \\
&\quad - \left(\frac{u_n-u_{n-1}}{h}\right)\frac{h^2}{8}V(x)v^{(+)}(x) - \frac{h^2}{24}\frac{\partial}{\partial x}\left(V(x)u(x)\right)\left(\frac{v_n^{(+)}+v_{n-1}^{(+)}}{2}\right) + \mathcal{O}(h^4) \\
&= \frac{u_{n-1}v_n^{(+)} - u_n v_{n-1}^{(+)}}{h} \\
&\quad + u(x)\frac{h^2}{24}\frac{\partial}{\partial x}\left(V(x)v^{(+)}(x)\right) + \frac{h^2}{8}V(x)u(x)\frac{\partial v^{(+)}(x)}{\partial x} \\
&\quad - \frac{\partial u(x)}{\partial x}\frac{h^2}{8}V(x)v^{(+)}(x) - \frac{h^2}{24}\frac{\partial}{\partial x}\left(V(x)u(x)\right)v^{(+)}(x) + \mathcal{O}(h^4) \\
&= \frac{u_{n-1}v_n^{(+)} - u_n v_{n-1}^{(+)}}{h} + \frac{h^2}{6}V(x)W(u,v^{(+)}) + \mathcal{O}(h^4) \qquad (66)
\end{aligned}
$$

Therefore we obtain

$$
W(u,v^{(+)}) = \frac{u_{n-1}v_n^{(+)} - u_n v_{n-1}^{(+)}}{h} + \frac{h^2}{6}V(x)W(u,v^{(+)}) + \mathcal{O}(h^4) \qquad (67)
$$

By recursively substituting the right-hand side into $W(u,v^{(+)})$ on the right-hand side of this equation, we obtain the following expression

$$
\begin{aligned}
W(u,v^{(+)}) &= \frac{u_{n-1}v_n^{(+)} - u_n v_{n-1}^{(+)}}{h} + \frac{h^2}{6}V(x)\left(\frac{u_{n-1}v_n^{(+)} - u_n v_{n-1}^{(+)}}{h} + \frac{h^2}{6}V(x)W(u,v^{(+)}) + \mathcal{O}(h^4)\right) + \mathcal{O}(h^4) \\
&= \left(1+\frac{h^2}{6}V(x)\right)\frac{u_{n-1}v_n^{(+)} - u_n v_{n-1}^{(+)}}{h} + \frac{h^4}{36}V^2(x)W(u,v^{(+)}) + \mathcal{O}(h^4) \qquad (68)
\end{aligned}
$$

Since the order of the second term on the right-hand side is h^4, it can be ignored as long as V(x) does not diverge. The $\frac{h^2}{6}V(x)$ in the first term on the right-hand side can be approximated using a finite difference representation with accuracy up to the third order, as

$$
\begin{aligned}
1+\frac{h^2}{6}V(x) &\approx 1+\frac{h^2}{6}\frac{V_n+V_{n-1}}{2} + \mathcal{O}(h^4) \\
&\approx \left(1+\frac{h^2}{12}V_n\right)\left(1+\frac{h^2}{12}V_{n-1}\right) + \mathcal{O}(h^4) \qquad (69)
\end{aligned}
$$

Thefore, using A_n defined by Eq.(13)

$$
W(u,v^{(+)}) = A_n A_{n-1}\frac{u_{n-1}v_n^{(+)} - u_n v_{n-1}^{(+)}}{h} + \mathcal{O}(h^4). \qquad (70)
$$

V. RENORMALIZED NUMEROV METHOD

The Renormalized Numerov method was developed by B. R. Johnson in 1977 [1]. This method is characterized by the following features:

- It utilizes the ratio of wave functions at adjacent mesh points instead of the wave function values themselves.
- It provides exceptional numerical stability against the exponential growth or decay of wave functions, effectively preventing overflow and underflow.
- It simplifies the handling of coupled-channel equations and the matching of boundary conditions.
- It preserves the fourth-order accuracy (with error of $\mathcal{O}(h^6)$) of the standard Numerov method.

In Eq.(15), if we define

$$F_n^{(\phi)} \equiv A_n \phi_n \tag{71}$$
$$U_n \equiv B_n / A_n \tag{72}$$

Eq.(15) can be rewritten as

$$F_{n+1}^{(\phi)} - U_n F_n^{(\phi)} + F_{n-1}^{(\phi)} = \mathcal{O}(h^6). \tag{73}$$

When solving the equation from the inside-out and when solving it from the outside-in, we define the ratios $R_n^{(\phi)}$ and $\widehat{R}_n^{(\phi)}$ as

$$R_n^{(\phi)} \equiv F_n^{(\phi)} / F_{n-1}^{(\phi)} \tag{74}$$
$$\widehat{R}_n^{(\phi)} \equiv R_n^{(\phi)-1} = F_{n-1}^{(\phi)} / F_n^{(\phi)} \tag{75}$$

respectively. Then Eq.(73) becomes

$$R_{n+1}^{(\phi)} - U_n + R_n^{(\phi)-1} = \mathcal{O}(h^6). \tag{76}$$

and

$$\widehat{R}_{n+1}^{(\phi)-1} - U_n + \widehat{R}_n^{(\phi)} = \mathcal{O}(h^6). \tag{77}$$

When solving the equation from the inside, if the wave function is zero at the origin ($\phi_0 = 0$), then $F_0^{(\phi)} = 0$, i.e. $R_1^{(\phi)-1} = 0$. Therefore, Eq.(76) for $n \geq 2$ can be solved recursively as

$$R_2^{(\phi)} = U_1 \tag{78}$$
$$R_3^{(\phi)} = U_2 - R_2^{(\phi)-1} \tag{79}$$
$$\vdots$$
$$R_N^{(\phi)} = U_{N-1} - R_{N-1}^{(\phi)-1}. \tag{80}$$

$F_1^{(\phi)}$ is given as an initial condition. By using Eq.(74), we can obtain $F_n^{(\phi)}$ for $n \geq 2$ as

$$F_2^{(\phi)} = R_2^{(\phi)} F_1^{(\phi)} \tag{81}$$
$$\vdots$$
$$F_N^{(\phi)} = R_N^{(\phi)} F_{N-1}^{(\phi)} \tag{82}$$

When solving the equation from the outside, one can give R_N^{out} from the given boundary conditions ϕ_N and ϕ_{N-1} as $\widehat{R}_N^{(\phi)} = F_{N-1}^{(\phi)} / F_N^{(\phi)}$. Then, for $n \leq N-1$, we can solve Eq.(77) recursively as

$$\widehat{R}_{N-1}^{(\phi)} = U_{N-1} - \widehat{R}_N^{(\phi)-1} \tag{83}$$
$$\widehat{R}_{N-2}^{(\phi)} = U_{N-2} - \widehat{R}_{N-1}^{(\phi)-1} \tag{84}$$
$$\vdots \tag{85}$$
$$\widehat{R}_1^{(\phi)} = U_1 - \widehat{R}_2^{(\phi)-1}. \tag{86}$$

By using Eq.(75), we can obtain $F_n^{(\phi)}$ for $n \leq N-2$ as

$$F_{N-2}^{(\phi)} = \widehat{R}_{N-1}^{(\phi)} F_{N-1}^{(\phi)} \tag{87}$$

$$\vdots$$

$$F_1^{(\phi)} = \widehat{R}_2^{(\phi)} F_2^{(\phi)}. \tag{88}$$

By using the solutions by the renormalized Numerov method, the Wronskian Eq.(70) can be rewritten as

$$W(u, v^{(+)}) = W_n = \frac{F_{n-1}^{(u)} F_n^{(v^{(+)})} - F_n^{(u)} F_{n-1}^{(v^{(+)})}}{h} + \mathcal{O}(h^4) \tag{89}$$

$$= \frac{1}{h} F_{n-1}^{(u)} F_n^{(v^{(+)})} \left(1 - R_n^{(u)} \widehat{R}_n^{(v^{(+)})}\right) + \mathcal{O}(h^4). \tag{90}$$

Since both $v^{(-)}$ and $v^{(+)}$ are obtained by solving from the outside, the Wronskian of $v^{(-)}$ and $v^{(+)}$ is as

$$W(v^{(-)}, v^{(+)}) = \frac{F_{n-1}^{(v^{(-)})} F_n^{(v^{(+)})} - F_n^{(v^{(-)})} F_{n-1}^{(v^{(+)})}}{h} + \mathcal{O}(h^4) \tag{91}$$

$$= \frac{1}{h} F_n^{(v^{(+)})} F_n^{(v^{(-)})} \left(\widehat{R}_n^{(v^{(-)})} - \widehat{R}_n^{(v^{(+)})}\right) + \mathcal{O}(h^4). \tag{92}$$

It should be noted that numerical instability may occur in the small r region, particularly when k is a large pure imaginary number ($k = i\kappa$ with $\kappa > 0$). In such cases, when integrating from the outside inward, one solution (e.g., $v^{(+)} \sim e^{-\kappa r}$) becomes dominant, while the other ($v^{(-)} \sim e^{\kappa r}$) becomes subdominant. Although the Renormalized Numerov method effectively prevents numerical overflow by utilizing the ratios of wave functions, it cannot entirely eliminate the loss of precision caused by the mixing of the dominant solution into the subdominant one. In the small r limit, both solutions are governed by the same irregular power-law behavior ($\sim r^{-l}$ for $l > 0$), which causes $\widehat{R}_n^{(v^{(-)})}$ to converge towards $\widehat{R}_n^{(v^{(+)})}$. As a result, the subtraction ($\widehat{R}_n^{(v^{(-)})} - \widehat{R}_n^{(v^{(+)})}$) in Eq.(92) suffers from a catastrophic cancellation of significant digits. Specifically, to avoid this cancellation, one can introduce the product of wave functions $G_n \equiv F_n^{(v^{(-)})} F_n^{(v^{(+)})}$. By utilizing Eq.(92), the unstable ratio $\widehat{R}_n^{(v^{(-)})}$ can be expressed as

$$\widehat{R}_n^{(v^{(-)})} = \widehat{R}_n^{(v^{(+)})} + \frac{hW}{G_n}. \tag{93}$$

Substituting this into the recurrence relation $G_{n-1} = \widehat{R}_n^{(v^{(-)})} \widehat{R}_n^{(v^{(+)})} G_n$, we obtain a stable propagation formula for G_n:

$$G_{n-1} = (\widehat{R}_n^{(v^{(+)})})^2 G_n + hW \widehat{R}_n^{(v^{(+)})}, \tag{94}$$

which enables the evaluation of the subdominant components solely in terms of the stable ratio $\widehat{R}_n^{(v^{(+)})}$ and the constant Wronskian W. Alternatively, since the Wronskian is analytically constant ($W = 2i/k$ for the Riccati-Hankel boundary conditions), its value evaluated at a stable point in the large r region can be utilized as a reliable reference for the entire coordinate range.

A. Coordinate independence of the Wronskian

The coordinate independence of the Wronskian can be seen by calculating $W_{n+1} - W_n$ using Eq.(89). From Eq.(89), we can obtain

$$W_{n+1} - W_n = \frac{1}{h}\left[\left(F_n^{(u)} F_{n+1}^{(v^{(+)})} - F_{n+1}^{(u)} F_n^{(v^{(+)})}\right) - \left(F_{n-1}^{(u)} F_n^{(v^{(+)})} - F_n^{(u)} F_{n-1}^{(v^{(+)})}\right)\right] + \mathcal{O}(h^4)$$

$$= \frac{1}{h}\left[F_n^{(u)}\left(F_{n+1}^{(v^{(+)})} + F_{n-1}^{(v^{(+)})}\right) - \left(F_{n+1}^{(u)} + F_{n-1}^{(u)}\right) F_n^{(v^{(+)})}\right] + \mathcal{O}(h^4) \tag{95}$$

By using Eq.(73), we can rewrite as

$$W_{n+1} - W_n = \frac{1}{h}\left[F_n^{(u)} U_n F_n^{(v^{(+)})} - F_n^{(u)} U_n F_n^{(v^{(+)})}\right] + \mathcal{O}(h^4) = 0. \tag{96}$$

While Eq.(96) theoretically proves the coordinate independence of the Wronskian, it also serves as a diagnostic for numerical instability. In the small r region with large pure imaginary k, the individual terms within the brackets of Eq.(96) can become extremely large due to the exponential growth of the dominant irregular solution. Consequently, the subtraction of these huge numbers leads to a catastrophic loss of significance (cancellation of significant digits), making the computed $W_{n+1} - W_n$ non-zero and highly unstable. This further clarifies the difficulty in maintaining the linear independence of two irregular solutions $v^{(+)}$ and $v^{(-)}$ in numerical practice. In contrast, the Wronskian $W(u, v^{(+)})$ used for the Jost function remains remarkably stable because the regular solution u vanishes at the origin, thereby suppressing the collision of large irregular components and preserving numerical precision even in the small r region.

[1] B. R. Johnson, J. Chem. Phys. **67**, 4086 (1977).