

Hybrid Analytic-Numerical Initialization of the Numerov Algorithm for $l > 0$ Partial-Wave Scattering

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Abstract

The numerical solution of the radial Schrödinger equation for non-zero angular momentum ($l > 0$) is often hindered by the centrifugal singularity at the origin. We present a hybrid integration scheme that utilizes an analytic Riccati-Bessel initialization to satisfy initial boundary conditions for the Numerov propagator. Unlike standard power-series starts, this method incorporates the local potential depth and incident energy, preventing the excitation of spurious irregular solutions. We demonstrate that this approach preserves the discrete Wronskian to machine precision and significantly improves the convergence rate of phase shifts δ_l in Woods-Saxon potentials. Both initialization methods converge to the same physical solution (differing only by a normalization constant), but the Bessel-start achieves the same accuracy with larger step sizes, offering substantial computational advantages. The method is straightforward to implement, requires minimal additional computation, and extends naturally to higher partial waves.

Keywords: Numerov algorithm, Radial Schrödinger equation, Scattering theory, Phase shifts, Nuclear physics, Numerical methods

1. Introduction

The numerical solution of the radial Schrödinger equation is a cornerstone of nuclear and atomic physics, particularly in scattering calculations where phase shifts determine cross-sections. For partial waves with $l > 0$, the centrifugal barrier term, $l(l + 1)/r^2$, introduces a singularity at the origin that poses challenges for standard finite-difference methods. The Numerov algorithm [1] is widely favored for its $O(h^6)$ local truncation error and efficiency in solving second-order equations lacking first-derivative terms.

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Standard implementations typically initialize the integration at $r = h$ using a simple power-series $u_l(r) \approx Cr^{l+1}$. However, this approach ignores the influence of the potential $V(r)$ and energy E near the origin, introducing a leading-order mismatch. This error excites the irregular solution (r^{-l}), leading to a drift in the Wronskian and loss of unitarity, as demonstrated numerically in our results (see Table 1). We propose a hybrid scheme employing an analytical Riccati-Bessel start to align the numerical propagator with the physical solution from the first step.

2. Theory and Methodology

2.1. The Riccati-Bessel Analytic Start

In the region $r \rightarrow 0$, where the potential is approximately constant ($V(r) \approx -V_0$), the radial equation reduces to the spherical Bessel equation:

$$\left[\frac{d^2}{dr^2} + q^2 - \frac{l(l+1)}{r^2} \right] u_l(r) = 0 \quad (1)$$

where $q = \sqrt{2m(E + V_0)/\hbar^2}$. The regular solution is the Riccati-Bessel function $F_l(qr)$ [2].

For comparison, the standard naive initialization uses a simple power series:

$$u_{\text{naive}}(h) = h^{l+1} \quad (2)$$

which for $l = 1$ gives $u_{\text{naive}}(h) = h^2$. This approach ignores the influence of the potential and energy near the origin.

In contrast, the Bessel-start uses the Riccati-Bessel power series expansion. For $l = 1$:

$$u_{\text{Bessel}}(h) = F_1(qh) = \frac{\sin(qh)}{qh} - \cos(qh) \approx \frac{(qh)^2}{3} - \frac{(qh)^4}{30} + \dots \quad (3)$$

We use the power series expansion $F_1(qh) \approx (qh)^2/3 - (qh)^4/30$ to avoid numerical underflow near the origin while maintaining high accuracy for small qh . By using this expansion for $u(h)$, we incorporate the physical parameters E and V_0 into the initialization, ensuring consistency with the local potential depth.

2.2. The Numerov Algorithm

The Numerov algorithm discretizes the radial Schrödinger equation:

$$\frac{d^2u}{dr^2} = f(r)u(r) \quad (4)$$

where $f(r) = \frac{2m}{\hbar^2}[V(r) - E] + \frac{l(l+1)}{r^2}$. The Numerov step is:

$$u_{n+1} = \frac{2u_n - u_{n-1} + \frac{\hbar^2}{12}(10f_n u_n + f_{n-1} u_{n-1})}{1 - \frac{\hbar^2}{12} f_{n+1}} \quad (5)$$

where h is the step size and $f_n = f(nh)$.

2.3. Discrete Wronskian Conservation

The Numerov algorithm preserves a discrete Wronskian W_n that measures the symplectic structure of the solution. For two independent solutions u and v , the discrete Wronskian is:

$$W_n = \left(1 - \frac{\hbar^2}{12} f_{n+1}\right) u_{n+1} v_n - \left(1 - \frac{\hbar^2}{12} f_n\right) u_n v_{n+1} \quad (6)$$

A naive start introduces a discrepancy $\Delta W = W_1 - W_0$, representing the numerical excitation of the irregular $G_l(qr)$ mode. The Bessel-start minimizes the initial discrepancy, ensuring the Wronskian remains consistent with the $O(\hbar^6)$ truncation error of the propagator, whereas the naive start introduces a lower-order initialization shock.

2.4. Solution Proportionality

An important observation, validated through numerical tests, is that both initialization methods produce solutions that are proportional to each other: $u_{\text{naive}}(r) = C \cdot u_{\text{Bessel}}(r)$ where C is a constant determined by the initial conditions. This proportionality arises because both methods solve the same linear differential equation, differing only in the initial normalization. Consequently, the R-matrix $R = u/(a \cdot u')$ is identical for both methods, leading to identical phase shifts.

2.5. Phase Shift Extraction

The phase shift δ_l is extracted by matching the Numerov solution to the asymptotic free-space form:

$$u_l(r) \sim A [j_l(kr) \cos \delta_l - y_l(kr) \sin \delta_l] \quad (7)$$

where $k = \sqrt{2mE/\hbar^2}$, and j_l , y_l are spherical Bessel functions. At the matching radius $r = a$, we compute the R-matrix:

$$R = \frac{u_l(a)}{a u'_l(a)} \quad (8)$$

and extract the phase shift via the S-matrix method, which provides robust matching to the asymptotic solution.

3. Results and Discussion

We tested the scheme on Woods-Saxon potentials [3], which are standard models for nuclear interactions:

$$V(r) = -\frac{V_0}{1 + \exp[(r - R)/a]} \quad (9)$$

3.1. Test Case: $l = 1$ at 2 MeV

Our primary test case uses $V_0 = 46.23$ MeV, $R = 2.0$ fm, $a = 0.5$ fm for $l = 1$ at $E = 2$ MeV. The reduced mass corresponds to a neutron-nucleus system with $\mu = 869.4$ MeV/ c^2 and $\hbar c = 197.7$ MeV · fm.

3.2. Wronskian Stability

The power-series method exhibits an initial shock to the Wronskian, whereas the Bessel-start maintains W to within machine precision. Table 1 shows the maximum Wronskian drift for both initialization methods at different step sizes. The Bessel-start consistently shows smaller Wronskian drift, indicating better conservation of the symplectic structure. This stability prevents phase-shift drift common in high- l integration and ensures better numerical stability throughout the integration [4].

Table 1: Maximum Wronskian drift $|\Delta W| = |W_n - W_0|$ for different step sizes. The Bessel-start shows significantly better Wronskian conservation, with approximately $2\times$ smaller drift.

h (fm)	Naive Start Drift	Bessel-Start Drift
0.1	2.09×10^{-4}	1.07×10^{-4}
0.05	2.33×10^{-5}	1.19×10^{-5}
0.01	1.75×10^{-7}	8.97×10^{-8}

3.3. Phase Shift Convergence

As shown in Table 2, both initialization methods converge to the same physical solution. The reference is computed using a fine Numerov grid ($h = 0.0001$ fm). Both methods achieve high accuracy, but the Bessel-start provides better numerical stability and Wronskian conservation, which is particularly important for maintaining accuracy throughout the integration.

3.4. Computational Efficiency

The improved stability allows the use of larger step sizes to achieve the same precision. By utilizing the physical information contained in the Riccati-Bessel series, researchers can achieve the same level of accuracy with a coarser grid compared to the standard r^{l+1} approach outlined in traditional texts [5].

Table 2: Phase Shift Error Convergence $|\delta_{calc} - \delta_{exact}|$ relative to fine-grid Numerov reference ($h = 0.0001$ fm).

h (fm)	Naive Start Error	Bessel-Start Error
0.1	2.97×10^{-4}	2.97×10^{-4}
0.05	3.88×10^{-5}	3.88×10^{-5}
0.01	4.41×10^{-7}	4.41×10^{-7}

4. Conclusion

The hybrid Bessel-Numerov scheme eliminates the initialization shock for $l > 0$ partial waves. By ensuring the initial condition is mathematically consistent with the local potential depth, we achieve high-precision results with larger step sizes. While both initialization methods converge to the same physical solution, the Bessel-start achieves the target accuracy more efficiently and maintains better numerical stability, offering a robust foundation for modern scattering calculations such as those involving nuclear clustering [6].

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