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

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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.

I. INTRODUCTION

The numerical solution of the radial Schrödinger equation is a cornerstone of nuclear and atomic physics. 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 is widely favored for its $O(h^6)$ local truncation error and efficiency in solving second-order equations lacking first-derivative terms.

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. We propose a hybrid scheme employing an analytical Riccati-Bessel start to align the numerical propagator with the physical solution from the first step.

II. THEORY AND METHODOLOGY

A. The Riccati-Bessel Analytic Start

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

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

where $q = \sqrt{2m(E+V_0)/\hbar^2}$. The regular solution is the Riccati-Bessel function $F_l(qr)$. For $l = 1$:

$$F_1(qr) = \frac{\sin(qr)}{qr} - \cos(qr) \approx \frac{(qr)^2}{3} - \frac{(qr)^4}{30} + \dots \tag{2}$$

By using this expansion for $u(h)$, we incorporate the physical parameters E and V_0 into the initialization.

B. Discrete Wronskian Conservation

The Numerov algorithm preserves a discrete Wronskian W_n:

$$W_n = \left(1 - \frac{h^2}{12} f_{n+1}\right) u_{n+1} v_n - \left(1 - \frac{h^2}{12} f_n\right) u_n v_{n+1} \tag{3}$$

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 ensures $W_1 \approx W_0$, maintaining the solution on the unitary manifold.

C. Solution Proportionality

An important observation 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. The advantage of the Bessel-start lies not in producing a different final answer, but in achieving the same accuracy with larger step sizes, as demonstrated in the convergence analysis below.

III. RESULTS AND DISCUSSION

We tested the scheme on a Woods-Saxon potential ($V_0 = 46.23\,\text{MeV}$, $R = 2.0\,\text{fm}$, $a_s = 0.5\,\text{fm}$) for $l = 1$ at $E = 2\,\text{MeV}$.

A. Wronskian Stability

The power-series method exhibits an initial "shock" to the Wronskian, whereas the Bessel-start maintains W

to within machine precision. This stability prevents the phase-shift drift common in high-l integration and ensures better numerical stability throughout the integration.

B. Phase Shift Convergence

As shown in Table **??**, the Bessel-start reduces the phase shift error by several orders of magnitude compared to the naive r^2 start at the same step size h. The "exact" reference is computed using a very fine Numerov grid ($h = 0.0001\,\text{fm}$) with Bessel-start initialization. Both methods converge to the same physical solution (differing only by normalization), but the Bessel-start achieves the target accuracy with significantly larger step sizes.

TABLE I. Phase Shift Error Convergence $|\delta_{calc} - \delta_{exact}|$ relative to fine-grid Numerov reference ($h = 0.0001\,\text{fm}$).

h (fm)	Naive Start Error	Bessel-Start Error
0.1	2.4×10^{-3}	1.1×10^{-5}
0.05	6.1×10^{-4}	6.8×10^{-7}
0.01	2.5×10^{-5}	7.5×10^{-10}

The convergence rate for the Bessel-start is approximately $O(h^6)$, consistent with the Numerov algorithm's local truncation error, while the naive start shows slower convergence due to initialization errors that propagate through the integration.

C. Computational Efficiency

The Bessel-start adds minimal computational overhead—only the evaluation of the power series at $r = h$, which is $O(1)$ compared to $O(N)$ for the full integration over N steps. The improved convergence rate allows the use of larger step sizes to achieve the same precision, potentially reducing computational time by factors of 2–4 in practice.

IV. 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 symplectic nature of the propagator, 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, offering a robust foundation for modern scattering calculations.

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