Comparison of Kohlrausch-Williams-Watts (KWW) and Havriliak-Negami (HN) Relaxation Models in the Context of Stevenson-Flux Information Theory (SFIT)

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Contents

1 Introduction

Relaxation phenomena in complex systems rarely follow simple exponential (Debye) decay. Two of the most important empirical models used to describe non-exponential relaxation are:

- The Kohlrausch–Williams–Watts (KWW) stretched exponential (time domain).
- The Havriliak–Negami (HN) function (frequency domain)[cite: 25, 26].

This document compares the two models mathematically and physically, with specific reference to their relevance in Stevenson-Flux Information Theory (SFIT) and the observed relaxation tails in the qBounce ILL 3-14-412 reanalysis.

2 Mathematical Definitions

2.1 Kohlrausch-Williams-Watts (KWW) Function

The KWW (stretched exponential) function in the time domain is:

$$\phi_{\mathrm{KWW}}(t) = A \exp\left[-\left(\frac{t}{\tau}\right)^{\beta}\right], \quad t \geq 0, \tag{1}$$

where A is the amplitude, τ is the characteristic relaxation time, and β is the stretching exponent ($0 < \beta \leq 1$). When $\beta = 1$, it reduces to a simple exponential. For $\beta < 1$, it produces a slower long-time tail[cite: 25, 26].

2.2 Havriliak-Negami (HN) Function

The HN model is defined in the frequency domain as the complex susceptibility:

$$\chi^*(\omega) = \frac{\Delta\chi}{[1 + (i\omega\tau)^{\alpha}]^{\gamma}}, \tag{2}$$

where $\Delta\chi$ is the relaxation strength, τ is the characteristic relaxation time, α is the symmetric broadening parameter ($0 < \alpha \leq 1$), and γ is the asymmetric broadening parameter ($0 < \gamma \leq 1$)[cite: 25].

Special cases include[cite: 25]:

- $\alpha = 1, \gamma = 1$: Debye (single exponential)[cite: 25].
- $\alpha = 1, \gamma = \beta$: Cole–Davidson (asymmetric)[cite: 25].
- $\alpha = \beta, \gamma = 1$: Cole–Cole (symmetric broadening)[cite: 25].
- General α, γ: Havriliak–Negami (most flexible)[cite: 25].

3 Key Comparison

Property	**KWW (Stretched Exponential)**	**Havriliak-Negami (HN)**
Domain	Time domain[cite: 25]	Frequency domain[cite: 25]
Primary Parameters	τ, β (1 parameter for shape)[cite: 25]	τ, α, γ (2 parameters for shape)[cite: 25]
Flexibility	Moderate[cite: 25]	High[cite: 25]
Typical Use	Time-resolved decay/relaxation tails[cite: 25]	Dielectric loss, impedance spectra[cite: 25, 26]
Physical Interpretation	Memory kernels/distributed relaxation[cite: 25, 26]	Broad distribution of relaxation times[cite: 25]
Fourier Transform	No simple closed form[cite: 25, 26]	Numerical Fourier transform needed[cite: 25, 26]
Limit $\beta, \alpha, \gamma \to 1$	Simple exponential[cite: 25]	Simple exponential (Debye)[cite: 25]

Table 1: Comparison of KWW and Havriliak-Negami models[cite: 25].

4 Advantages and Limitations

4.1 KWW Advantages

- Simple single shape parameter β[cite: 25].
- Directly applicable to time-domain data (e.g., post-mirror-step relaxation in qBounce)[cite: 25].
- Easy to interpret in terms of memory effects or heterogeneous relaxation[cite: 25, 26].
- Computationally lightweight for fitting time series[cite: 25].

4.2 KWW Limitations

- Less flexible than HN for describing both symmetric and asymmetric broadening[cite: 25].
- Fourier transform lacks closed form, complicating frequency-domain comparisons[cite: 25, 26].
- Can fail at very short or extremely long times[cite: 25, 26].

4.3 HN Advantages

- More flexible; can model both symmetric (α) and asymmetric (γ) broadening simultaneously[cite: 25].
- Naturally suited for frequency-domain data (impedance, dielectric loss spectra)[cite: 25, 26].
- Reduces to several well-known special cases (Cole–Cole, Cole–Davidson, Debye)[cite: 25].

4.4 HN Limitations

- Two shape parameters make fitting more ambiguous and prone to parameter correlation[cite: 25].
- Less intuitive for direct time-domain relaxation tails[cite: 25].
- Requires numerical Fourier transform to compare with time-domain experiments[cite: 25, 26].

5 Relevance to SFIT and qBounce Data

In Stevenson-Flux Information Theory (SFIT), the observed relaxation tails after mirror steps in the ILL 3-14-412 dataset are well-described by a KWW function with[cite: 25]:

$$\tau \approx 832.6 \text{ s}, \quad \beta = 1.060 = K, \tag{3}$$

where K is the refined coupling kernel[cite: 25].

The KWW model is preferred here for the following reasons[cite: 25]:

- The data is primarily time-domain (event-by-event timestamps after mirror steps)[cite: 25].
- The single stretching parameter β has a clear physical mapping to the SFIT coupling kernel $K = 1.060$[cite: 25].

- The memory kernel induced by the 1.20134 mHz information flux naturally produces a stretched-exponential form in the time domain[cite: 25, 26].
- The synthetic data generator and analyzer scripts successfully recover τ and β close to theoretical values[cite: 25].

While the Havriliak–Negami model offers greater flexibility in frequency domain, it would introduce an unnecessary second shape parameter without clear physical justification in the current SFIT framework[cite: 25, 26]. If future frequency-domain measurements (e.g., resonant spectroscopy) become available, HN could be explored as a complementary description[cite: 25, 26].

6 When to Choose Which Model?

- Use KWW when working with direct time-resolved decay data and a single stretching mechanism is physically motivated (as in SFIT)[cite: 25, 26].
- Use HN when analyzing frequency-domain spectra with both symmetric and asymmetric broadening, or when high fitting flexibility is required[cite: 25, 26].

In many real systems, KWW and HN are approximately related through numerical Fourier transforms, allowing conversions between time and frequency responses[cite: 25, 26].

7 Conclusion

The KWW function provides a simple, physically motivated description of the relaxation tails in SFIT, directly linking the stretching exponent β to the coupling kernel K[cite: 25]. While the Havriliak–Negami model is more general and flexible in the frequency domain, KWW is more appropriate and parsimonious for the time-domain qBounce residuals and the dynamic flux model of gravity[cite: 25].

Both models ultimately point to underlying distributions of relaxation times or memory effects—phenomena that SFIT explains through the oscillatory information-carrying gravitational flux at 1.20134 mHz[cite: 25].

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