

CTMT: Full Elemental Computation

Phase-Aware Kernel, Fisher Geometry, Rupture, and Groupwise Constraints with Dimensional Closure

Matěj Rada Email: MatejRada@email.cz

This work is licensed under a Creative Commons Attribution–NonCommercial–NoDerivatives 4.0 License.

Abstract

This document presents the current consolidated formulation of the *Chronotopic Theory of Matter and Time* (CTMT) for elemental-scale computation across atomic number Z . We specify a bona fide phase channel within the kernel, define the likelihood and Fisher geometry under dimensional closure, and provide the inversion scheme (Gauss–Newton with damping) together with rupture analysis on phase-rich observables. Groupwise regularity (including lanthanide contraction with endpoint anchoring) and admissibility of mass modulation in the presence of phase sensitivity are formalized. Beyond formal definitions, an appendix documents the *execution trace*: step-by-step numerical operations where causality, phase, Fisher geometry, and rupture are computed. Citations are provided to standard references for Fisher information, robust statistics, and Gauss–Newton damping.

Contents

1 Scope and Minimal Assumptions	2
2 Kernel with a Bona Fide Phase Channel	2
2.1 Phase Sensitivity and Measurability	2
2.2 Frequency-Domain Representation	2
3 Forward Model, Observables, and Likelihood	3
4 Fisher Geometry and Identifiability	3
4.1 Elemental Fisher Trajectory	3
5 Inversion: Gauss–Newton with Damping	3
6 Conjugate Recovery and Mass Modulation	4
6.1 Admissibility of Mass Modulation (AAA)	4
7 Rupture Analysis on Phase-Rich Spectra	4
8 Groupwise Structure and Regularization	4
8.1 Lanthanide Contraction	4
9 Dimensional Closure	5
10 Computation Over Elements	5
11 Acceptance Criteria	5
A Execution Trace: Step-by-Step Guidance	5

1 Scope and Minimal Assumptions

We consider a collection of elements indexed by atomic number $Z \in \mathcal{Z} \subset \mathbb{Z}_{>0}$ and a set of experiments producing observables $\mathcal{O}(Z) \in \mathbb{R}^m$ under a forward operator determined by a kernel with amplitude and phase structure. CTMT imposes **dimensional closure**—all terms entering the objective are dimensionless or integrated with unit-canceling measures—and a **closed topology** under which admissible transformations preserve identifiability and causality.

Definition 1 (Element index set). The elemental index set is $\mathcal{Z} = \{Z_1, Z_2, \dots, Z_n\} \subset \mathbb{Z}_{>0}$, equipped with the natural order and any physically relevant partition into chemical groups.

Assumption 1 (Minimal structure). (A1) **Kernel regularity:** The kernel \mathcal{K} is measurable on a time domain $\mathcal{T} \times \mathcal{T}$ with $\mathcal{T} \subset \mathbb{R}$, causal in the sense that it has negligible support for $t < t'$, and decomposes into amplitude and phase channels (Section 2).

- (A2) **Noise model:** Measurement noise is zero-mean with known or estimable covariance Σ , and independent across experiments conditional on parameters (Section 3).
- (A3) **Phase sensitivity:** The phase channel $\Phi(t, t')$ satisfies $\partial_{t'} \Phi \neq 0$ on a set of non-zero measure within $\mathcal{T} \times \mathcal{T}$ (Section 2.1).
- (A4) **Dimensional closure:** All objective terms are rendered dimensionless either by reference scaling, integration against appropriate measures, or normalization by Fisher-consistent factors (Section 9).

2 Kernel with a Bona Fide Phase Channel

Let $\mathcal{K} : \mathcal{T} \times \mathcal{T} \rightarrow$ be written as

$$\mathcal{K}(t, t'; \vartheta) = A(t, t'; \vartheta) \exp(i \Phi(t, t'; \vartheta)), \quad (1)$$

where $A \geq 0$ is a real-valued amplitude channel and Φ is a real-valued phase channel. The parameter set ϑ may include dispersion coefficients and couplings to element-level latent variables.

2.1 Phase Sensitivity and Measurability

We require that Φ be *measurably sensitive* to its second argument in the sense that

$$\mu(\{(t, t') \in \mathcal{T}^2 : |\partial_{t'} \Phi(t, t'; \vartheta)| > \epsilon\}) > 0 \quad \text{for some } \epsilon > 0, \quad (2)$$

where μ is the product measure on \mathcal{T}^2 . This condition allows recovery of conjugate quantities (§6) and renders mass modulation admissible within CTMT (§6.1).

2.2 Frequency-Domain Representation

Assuming \mathcal{K} is L^2 in both variables and sufficiently decaying, define the partial Fourier transform in $(t - t')$ and denote frequency by Ω :

$$\widehat{\mathcal{K}}(\Omega; t') = \int_{\mathcal{T}} \mathcal{K}(t, t') e^{-i\Omega(t-t')} dt. \quad (3)$$

A dispersive mapping $k(\Omega)$ may be embedded via $\Phi(t, t') = \int_{t'}^t \Omega(\tau) d\tau$ with $\Omega \mapsto k(\Omega)$ tied to an observable such as spectral phase or group delay.

3 Forward Model, Observables, and Likelihood

Let $x(Z) \in \mathbb{R}^p$ denote element-resolved latent parameters (e.g., radii, masses, couplings). Observables $\mathcal{O}(Z) \in \mathbb{R}^m$ are generated by

$$\mathcal{O}(Z) = H(x(Z); \mathcal{K}(\cdot, \cdot; \vartheta)) + \eta, \quad \eta \sim \mathcal{N}(0, \Sigma), \quad (4)$$

where H integrates the kernel against experiment-specific probes. Split \mathcal{O} into *monotone* channels (e.g., $\kappa \propto Z$, diffusivities) and at least one *phase-linked* non-monotone observable, O_{phase} , such as coherence length or spectral phase curvature.

Given independent experiments indexed by i , the negative log-likelihood (NLL) obeys dimensional closure by either scaling or normalizing each channel:

$$\mathcal{L}(x, \vartheta) = \frac{1}{2} \sum_{Z \in \mathcal{Z}} \sum_i \|W_i^{1/2} (\mathcal{O}_i^{\text{meas}}(Z) - \mathcal{O}_i^{\text{mod}}(Z; x, \vartheta))\|_2^2 + \mathcal{R}(x, \vartheta), \quad (5)$$

with W_i dimensionless weights (often Σ_i^{-1} post-normalization) and \mathcal{R} an admissible regularizer (§8).

4 Fisher Geometry and Identifiability

Let θ collect all free parameters in $\{x(Z)\}_{Z \in \mathcal{Z}}$ and ϑ . The (expected) Fisher information matrix (FIM) is

$$\mathcal{F}(\theta) = \mathbb{E} \left[\nabla_\theta \log p(\mathcal{D} | \theta) \nabla_\theta \log p(\mathcal{D} | \theta)^\top \right] \approx J(\theta)^\top W J(\theta), \quad (6)$$

where J is the Jacobian of residuals [1]. CTMT favors *isotropic* Fisher spectra along the inversion path; thus, we **rebalance** the observable set to avoid dominance by monotone channels, improving conditioning and Gauss–Newton performance.

Proposition 1 (Phase channel improves local conditioning). If O_{phase} is informative with non-collinear sensitivity to x , then the smallest eigenvalue of \mathcal{F} increases under its inclusion, reducing the condition number $\kappa(\mathcal{F})$ provided W is scaled under closure.

4.1 Elemental Fisher Trajectory

Across atomic number, CTMT monitors the Fisher spectrum as a function of Z :

$$\lambda_{\min}(Z), \quad \kappa(Z) = \frac{\lambda_{\max}(Z)}{\lambda_{\min}(Z)}. \quad (7)$$

Stable elemental computation requires bounded $\kappa(Z)$ under (i) reweighting of monotone observables, (ii) inclusion/exclusion of the phase channel, and (iii) moderate regularization changes. Sharp increases in $\kappa(Z)$ indicate loss of causal identifiability and precede observable rupture in $Y(Z)$.

5 Inversion: Gauss–Newton with Damping

Define residuals $r(\theta) = W^{1/2}(\mathcal{O}^{\text{meas}} - \mathcal{O}^{\text{mod}})$ and $J = \partial r / \partial \theta$. One step of damped Gauss–Newton (GN) solves

$$(J^\top J + \lambda I) \Delta \theta = -J^\top r, \quad \theta_{k+1} = \theta_k + \Delta \theta, \quad (8)$$

with Levenberg–Marquardt damping $\lambda \geq 0$ [2, 3]. Convergence is declared when $\|\Delta \theta\|$ and the reduction in \mathcal{L} fall below tolerance. Success rates improve materially after rebalancing with O_{phase} .

6 Conjugate Recovery and Mass Modulation

Consider a conjugate quantity S_* (e.g., an effective source) linked to the phase-bearing kernel via a linear operator \mathcal{A} on the same grid:

$$\mathcal{A}[S_*](t) = \int_{\mathcal{T}} \mathcal{K}(t, t') S_*(t') dt'. \quad (9)$$

Proposition 2 (S^* recovery under phase sensitivity). If (2) holds and $A(t, t')$ is non-degenerate on the support of S_* , then S_* is identifiable (up to null-space symmetries) from phase-bearing observables, with stability governed by the Fisher spectrum of the induced linearized map.

6.1 Admissibility of Mass Modulation (AAA)

Mass (or mass-like) modulation of a component AAA is admissible under CTMT only when the kernel carries a measurable phase channel per (2); otherwise the modulation is declined as non-identifiable under closure. With phase present, modulation parameters enter θ and are regularized by Fisher-consistent priors.

7 Rupture Analysis on Phase-Rich Spectra

Let $Y(Z)$ denote a scalar phase-linked observable across elements. We define a robust rupture score using standardized second differences:

$$R(Z_k) = \frac{\Delta^2 Y(Z_k) - \text{med}(\Delta^2 Y)}{1.4826 \text{ med} |\Delta^2 Y - \text{med}(\Delta^2 Y)|}, \quad \Delta^2 Y(Z_k) = Y(Z_{k+1}) - 2Y(Z_k) + Y(Z_{k-1}). \quad (10)$$

This statistic uses the median and MAD for robustness to outliers [4]. Kinks (change-points) satisfy $|R(Z_k)| > \tau$ with $\tau \approx 3.5$ and are validated by robustness to rebinning and mild regularization changes.

8 Groupwise Structure and Regularization

Partition \mathcal{Z} into chemical groups G_g (alkali, alkaline earth, transitions, pnictogens, chalcogens, halogens, noble gases, lanthanides, actinides). For a parameter field $x(Z)$ we impose piecewise-smooth priors with optional endpoint anchoring:

$$\mathcal{R}(x) = \sum_g \alpha_g \sum_{Z \in G_g} (\nabla_Z x(Z))^2 + \sum_{(Z_a, Z_b) \in \mathcal{A}} \beta_{ab} (x(Z_a) - x_a^\circ)^2 + (x(Z_b) - x_b^\circ)^2, \quad (11)$$

where \mathcal{A} collects anchored endpoints (Z_a, Z_b) with targets x° .

8.1 Lanthanide Contraction

For $Z = 57 \dots 71$, we enforce endpoint anchoring and monotone curvature consistent with CTMT rigidity:

$$\Delta_Z x(Z) < 0 \quad \text{for successive } Z, \quad x(57) = x_{\text{La}}^\circ, \quad x(71) = x_{\text{Lu}}^\circ. \quad (12)$$

External validation can be performed against Shannon ionic radii at coordination number 8; errors are summarized by

$$\text{MAE} = \frac{1}{n} \sum_k |x(Z_k) - x_{\text{ref}}(Z_k)|, \quad \text{RMSE} = \sqrt{\frac{1}{n} \sum_k (x(Z_k) - x_{\text{ref}}(Z_k))^2}. \quad (13)$$

For reference data, see [5].

9 Dimensional Closure

CTMT requires that each cost term be dimensionless or accompanied by a unit-canceling measure. Typical strategies include: (i) normalizing observables by reference scales, (ii) prewhitening with physically grounded W , (iii) scaling regularization by Fisher-consistent factors so that \mathcal{L} is unitless. This extends to all regimes and entities in the ontology, not only specific measurement protocols.

10 Computation Over Elements

For each $Z \in \mathcal{Z}$:

1. Assemble $\mathcal{O}(Z)$ including at least one phase-linked observable O_{phase} .
2. Evaluate residuals and Jacobians under (5), enforcing closure.
3. Update θ via (8) with trust adjustment of λ .
4. Monitor Fisher spectra and condition numbers; if anisotropy emerges, rebalance weights or augment observables.
5. Compute rupture score (10) on phase-rich series $Y(Z)$; register kinks.
6. Apply groupwise constraints (11); in lanthanides, enforce (12).

11 Acceptance Criteria

A solution is accepted if:

- (C1) **Phase channel:** $\partial_{t'}\Phi \neq 0$ on non-zero measure; S_* reconstruction on the kernel grid attains finite error bounded by Fisher conditioning.
- (C2) **Fisher isotropy:** Inclusion of O_{phase} reduces $\kappa(\mathcal{F})$ relative to baseline and improves Gauss–Newton success rate.
- (C3) **Rupture:** $R(Z)$ reveals stable kinks around physically expected regions (e.g., radioactives) with robustness to smoothing.
- (C4) **Lanthanides:** Contraction monotonicity holds under endpoint anchoring; external MAE/RMSE are within admissible bounds.
- (C5) **Closure:** The complete objective remains dimensionless; any mass modulation parameters are admissible only with the verified phase channel.

A Execution Trace: Step-by-Step Guidance

This appendix translates the formal sections into a minimal execution trace for CTMT elemental computation.

Step 1: Kernel Instantiation (Causality + Phase)

For fixed Z , define $\mathcal{K}_Z(t, t') = A_Z(t, t') e^{i\Phi_Z(t, t')}$. Numerically tabulate or parameterize A_Z and Φ_Z . Verify phase sensitivity: $\partial_{t'}\Phi_Z \neq 0$ on non-zero measure (Section 2.1). If this fails, CTMT halts and any mass modulation is forbidden (Section 6.1).

Step 2: Observable Synthesis

Compute $\mathcal{O}(Z) = H(x(Z); \mathcal{K}_Z)$, ensuring at least one *phase-linked* observable depends non-linearly on Φ_Z ; others may be monotone. This asymmetry is intentional to improve Fisher conditioning (Sections 3 and 4).

Step 3: Dimensionally Closed Residuals

Form residuals $r_i(Z) = W_i^{1/2}(\mathcal{O}_i^{\text{meas}}(Z) - \mathcal{O}_i^{\text{mod}}(Z))$ with W_i chosen to enforce dimensional closure (Section 9). Reject any term with hidden unit leakage.

Step 4: Fisher Geometry Construction

Compute the Jacobian $J_Z = \partial r(Z)/\partial \theta$ and the Fisher matrix $\mathcal{F}_Z = J_Z^\top J_Z$ [1]. Test: full rank, acceptable isotropy, and whether adding the phase observable increases $\lambda_{\min}(\mathcal{F}_Z)$.

Step 5: Gauss–Newton Update (Conditional)

Only if Fisher geometry passes, solve $(J^\top J + \lambda I)\Delta\theta = -J^\top r$ with Levenberg–Marquardt damping $\lambda \geq 0$ [2, 3]. GN is subordinate to Fisher geometry; degrade *or* damp updates if conditioning worsens.

Step 6: Rupture Computation (Across Z)

After sweeping Z , compute $R(Z)$ per (10). Interpret large $|R(Z)|$ as a break in transport coherence (structural change), not mere fit error. Validate kinks by robustness checks [4].

Step 7: Groupwise Enforcement

Apply constraints such as $\Delta_Z x(Z) < 0$ in lanthanides (Section 8). Treat these as CTMT closure conditions justified by Fisher rigidity, not arbitrary priors.

B Minimal Elemental Computation Loop (Pseudo-code)

```

for Z in Z_set:
    K = build_kernel(A_Z, Phi_Z)                  # Check causality; verify d/dt' Phi_Z != 0
    O_mod = forward_model(x[Z], K)                # Includes at least one phase-linked observable
    r = W_sqrt @ (O_meas[Z] - O_mod)              # Closure: r is dimensionless
    J = jacobian(r, theta)                        # Numeric differentiation or adjoint
    F = J.T @ J                                    # Fisher geometry
    if passes_geometry(F):
        dtheta = solve((J.T@J + lambda*I) * dtheta == -J.T * r) # LM damping
        theta = update(theta, dtheta)
    else:
        adjust_weights_or_observables()
# Across Z: rupture on phase-rich series
R = robust_second_diff(Y_by_Z)                  # median/MAD standardized
kinks = { Z: abs(R[Z]) > 3.5 }
# Enforce groupwise constraints
apply_groupwise_constraints(x)

```

References

- [1] R. A. Fisher, “Theory of statistical estimation,” *Proceedings of the Cambridge Philosophical Society*, vol. 22, pp. 700–725, 1925.

- [2] K. Levenberg, “A method for the solution of certain non-linear problems in least squares,” *Quarterly of Applied Mathematics*, vol. 2, pp. 164–168, 1944.
- [3] D. W. Marquardt, “An algorithm for least-squares estimation of nonlinear parameters,” *SIAM Journal on Applied Mathematics*, vol. 11, no. 2, pp. 431–441, 1963.
- [4] P. J. Huber and E. M. Ronchetti, *Robust Statistics*, 2nd ed., Wiley, 2009.
- [5] R. D. Shannon, “Revised effective ionic radii and systematic studies of interatomic distances in halides and chalcogenides,” *Acta Crystallographica Section A*, vol. 32, pp. 751–767, 1976.