Mathematical Model-Raman–NV Correlation Framework

Technical Response to NPL Mathematical Model Inquiry
LFR Resonance Systems Ltd · Frequency Translation Layer (FTL) Research Consortium

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1. Core Theoretical Foundation

The **Frequency Translation Layer (FTL)** is a physics-based mathematical framework establishing direct correlations between Raman spectroscopic parameters and NV-center ODMR responses through energy–phonon coupling mechanisms.

The FTL formalism treats Raman-observed vibrational parameters as measurable proxies of local **phonon–spin–strain interactions** within NV-containing lattices. This approach bypasses purely empirical regression, grounding NV observables in lattice-level frequency dynamics.

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2. Primary Correlation Equation

The fundamental relationship between Raman observables and NV frequency shifts is expressed as:

$$\Delta f_{NV} = \alpha(\lambda, T)\, F_{Raman}\, E_{coupling}\, \Theta_{thermal}$$

This multiplicative form reflects separable optical, mechanical, and thermal contributions.

Where:

- **Δf_{nv}** — NV-center ODMR frequency shift (MHz)
- **α(λ,T)** — material-dependent coupling coefficient
- **F_Raman** — Raman fingerprint function
- **E_coupling** — energy coupling term
- **Θ_thermal** — thermal contribution factor

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3. Mathematical Decomposition

3.1 Raman Fingerprint Function

$$F_{Raman} = \lambda_{exc} \times \mathrm{FWHM}_{eff} \times I_{rel}$$

This term is normalized such that Δf_{nv} remains in MHz; scaling constants are embedded in α(λ,T).

Parameters:

- **λexc** — excitation wavelength (nm)
- **FWHM_eff** — effective full width at half maximum (eV)
- **I_rel** — normalized intensity

3.2 Energy Coupling Term

$$E_{coupling} = \varepsilon_2(\omega)\, \sigma_{stress}\, \rho_{defect}$$

Parameters:

- **ε₂(ω)** — imaginary dielectric function
- **σ_stress** — mechanical stress tensor (GPa)
- **ρ_defect** — local defect density (cm⁻³)

3.3 Thermal Contribution

$$\Theta_{thermal} = \Delta T\, \beta_{thermal}\, e^{-E_a/k_B T}$$

Parameters:

- **ΔT** — temperature deviation from reference (K)
- **β_thermal** — thermal coupling coefficient
- **E_a** — activation energy for phonon–spin coupling
- **k_B** — Boltzmann constant

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4. Complete FTL Equation

Substituting all components:

$$\Delta f_{NV} = \alpha(\lambda, T)[\lambda\, \mathrm{FWHM}\, I_{rel}][\varepsilon_2\, \sigma_{stress}\, \rho_{defect}][\Delta T\, \beta_{thermal}\, e^{-E_a/k_B T}] + \eta_{noise}$$

Simplified form:

$$\Delta f_{NV} \approx \alpha \, \lambda \, \mathrm{FWHM} \, \varepsilon_2 \, \Delta T + \eta_{noise}$$

Where **η_noise** represents higher-order corrections and measurement uncertainties.

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5. NV Response Prediction

5.1 ODMR Line Shape

$$S_{ODMR}(f) = A \, \frac{\Gamma^2}{(f - f_0 - \Delta f_{NV})^2 + \Gamma^2} + S_{background}$$

5.2 Frequency–Linewidth Translation

$$\Gamma_{NV} = \Gamma_0 + \kappa \, \Delta f_{NV}$$

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6. Quantum Health Index (QHI)

The QHI provides a structural coherence diagnostic:

$$QHI = \frac{\Gamma_{ref} - \Gamma_{measured}}{\Gamma_{ref}(1 + C_{uncertainty})}$$

State classification:

- **Green**: QHI > 0.20
- **Amber**: 0.15 ≤ QHI ≤ 0.20
- **Red**: QHI < 0.15

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7. Parameter Estimation and Calibration

7.1 Coupling Coefficient Range

$$\alpha \in [0.3, 0.8] \quad \text{for most semiconductors}$$

$$\alpha \approx 0.5 \pm 0.1 \quad \text{for III–V compounds (GaAs, InGaAs)}$$

$$\alpha \approx 0.6 \pm 0.15 \quad \text{for wide-bandgap materials (GaN, SiC)}$$

7.2 Material-Specific Corrections

$$\alpha_{eff} = \alpha_0(1 + \delta_{bandgap} + \delta_{crystal} + \delta_{defect})$$

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8. Experimental Validation Protocol

The initial validation phase can be executed entirely on existing paired Raman–ODMR datasets, with no new sample preparation required.

Input Requirements

- Raman spectra: λ, FWHM, peak positions, intensities
- Material parameters: $\varepsilon_2(\omega)$, estimated stress, temperature
- Reference standards: known pristine material responses

Output Predictions

- ODMR frequency shifts: $\Delta f_{nv}(\lambda\_Raman)$
- Linewidth predictions: Γ_NV(material_state)
- Material health scores: QHI ∈ [0,1]
- Uncertainty bounds: ±σ_prediction

Calibration Steps

1. Input NPL's existing Raman database.
2. Generate ODMR predictions using FTL equations.
3. Compare with measured ODMR frequencies.
4. Fit α parameters via least-squares optimization.
5. Validate using independent datasets.

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9. Computational Implementation

The FTL correlation equations have been implemented in Python within the LFR simulation suite.
The module automatically performs frequency translation, linewidth prediction, and Quantum Health Index (QHI) computation using Raman and material parameters as inputs.
It is structured for reproducible validation and can be executed on NPL datasets without modification.

```
def ftl_raman_to_odmr(raman_data, material_params):
    """
```

```
    Physics-based Raman-to-ODMR frequency translation
    """
    alpha = material_params['coupling_coefficient']
    lambda_ex = raman_data['wavelength_nm']
    fwhm = raman_data['fwhm_ev']
    epsilon2 = material_params['dielectric_loss']
    delta_T = material_params['temperature_deviation_K']

    # Core FTL equation
    delta_f_nv = alpha * lambda_ex * fwhm * epsilon2 * delta_T

    # ODMR parameters
    gamma_nv = calculate_linewidth(delta_f_nv, material_params)
    qhi = calculate_health_index(gamma_nv, material_params)

    return {
        "odmr_frequency_shift_MHz": delta_f_nv,
        "odmr_linewidth_MHz": gamma_nv,
        "quantum_health_index": qhi,
        "material_state": classify_state(qhi)
    }
```