Quantum Phase MRI Simulation: Finite Mathematics & Circuit Derivations

NeuroPulse Physics Engine v3.0
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Executive Summary

This report presents the complete finite mathematical framework for quantum phase-based MRI reconstruction, including discrete Bloch equation solutions, RF coil circuit topology derivations, and Berry phase accumulation in topological pulse sequences. All derivations are presented in discrete form suitable for numerical implementation.

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1. Discrete Bloch Equations for Quantum Phase Evolution

1.1 Finite Difference Formulation

The continuous Bloch equations are discretized using forward Euler method with time step Δt:

$$M_x^{n+1} = M_x^n + \Delta t\left[\gamma\,(M_y^n B_z - M_z^n B_y) - \frac{M_x^n}{T_2}\right]$$

$$M_y^{n+1} = M_y^n + \Delta t\left[\gamma\,(M_z^n B_x - M_x^n B_z) - \frac{M_y^n}{T_2}\right]$$

$$M_z^{n+1} = M_z^n + \Delta t\left[\gamma\,(M_x^n B_y - M_y^n B_x) - \frac{M_z^n - M_0}{T_1}\right]$$

where: - $M^n = (M_x^n, M_y^n, M_z^n)$ is the magnetization vector at time step n - $\gamma = 42.58$ MHz/T is the gyromagnetic ratio - $B = (B_x, B_y, B_z)$ is the magnetic field vector - T_1, T_2 are relaxation time constants

1.2 Stability Criterion

For numerical stability, the time step must satisfy:

$$\Delta t < \frac{2}{\gamma\,B_{\max} + \max(1/T_1, 1/T_2)}$$

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2. Quantum Berry Phase Accumulation

2.1 Geometric Phase in Parameter Space

The Berry phase γ_B accumulated during adiabatic evolution along a closed path C in parameter space is:

$$\gamma_B(C) = i_C \langle \psi_n(\mathbf{R}) | \nabla_{\mathbf{R}} | \psi_n(\mathbf{R}) \rangle \cdot d\mathbf{R}$$

For MRI applications with spatially varying gradients, this becomes:

$$\gamma_B(\mathbf{r}) = \int_0^T \mathbf{A}(\mathbf{r}, t) \cdot \frac{d\mathbf{r}}{dt} \, dt$$

where $\mathbf{A}$ is the Berry connection (gauge potential).

2.2 Discrete Berry Phase Calculation

In discrete form with N time steps:

$$\gamma_B \approx \sum_{n=0}^{N-1} \mathbf{A}_n \cdot \Delta \mathbf{r}_n$$

where:

$$\mathbf{A}_n = \text{Im}\left[\langle \psi_n | \frac{\psi_{n+1} - \psi_n}{\Delta t} \rangle \right]$$

2.3 Berry Curvature and Topological Invariant

The Berry curvature tensor is:

$$\Omega_{ij}(\mathbf{k}) = \partial_{k_i} A_j - \partial_{k_j} A_i$$

The Chern number (topological invariant) is:

$$C = \frac{1}{2\pi} \int_{BZ} \Omega_{xy}(\mathbf{k}) d^2 k$$

For discrete k-space sampling on an $N \times N$ grid:

$$C \approx \frac{1}{2\pi} \sum_{i=1}^{N} \sum_{j=1}^{N} \Omega_{xy}(k_i, k_j) \Delta k_x \Delta k_y$$

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3. RF Coil Circuit Topology

3.1 Birdcage Coil Impedance Matrix

For an N-rung birdcage coil, the impedance matrix $\mathbf{Z}$ is:

$$Z_{ij} = \begin{cases} R + j\omega L_{leg} + \dfrac{1}{j\omega C_{ring}} & i = j \\[2ex] \dfrac{1}{j\omega C_{ring}} & |i-j| = 1 \text{ or } N-1 \\[2ex] 0 & \text{otherwise} \end{cases}$$

The resonant frequencies are:

$$\omega_m = \frac{1}{\sqrt{L_{leg} C_{ring}}} \, 2 \sin\left(\frac{m\pi}{N} \right)^{-1}, \quad m = 1, 2, \cdots, N/2$$

3.2 Mutual Inductance Calculation

For two circular loops with radii a_1, a_2 separated by distance d:

$$M_{12} = \mu_0\sqrt{a_1 a_2}\left[\left(2-k^2\right)K(k)-2E(k)\right]$$

where: - $k^2 = \dfrac{4a_1 a_2}{(a_1 + a_2)^2 + d^2}$ - $K(k), E(k)$ are complete elliptic integrals

Discrete approximation using mesh elements:

$$M_{ij} \approx \sum_{p=1}^{N_1} \sum_{q=1}^{N_2} \frac{\mu_0}{4\pi} \frac{\mathbf{J}_i^p \cdot \mathbf{J}_j^q}{|\mathbf{r}_{ij}^{pq}|} \Delta A_p \Delta A_q$$

3.3 Quantum Surface Lattice Coupling

For a hexagonal lattice of quantum coil elements, the coupling Hamiltonian is:

$$H_{coupling} = \sum_{\langle i,j \rangle} J_{ij}(\sigma_i^+ \sigma_j^- + \sigma_i^- \sigma_j^+) + \sum_i h_i \sigma_i^z$$

The flux quantization condition:

$$\Phi = n\Phi_0, \quad \Phi_0 = \frac{h}{2e} = 2.067 \times 10^{-15} \text{ Wb}$$

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4. K-Space Trajectory and Reconstruction

4.1 Discrete Fourier Transform

The k-space signal is related to the image by discrete Fourier transform:

$$S(k_x, k_y) = \sum_{m=0}^{M-1} \sum_{n=0}^{N-1} \rho(m, n)e^{-2\pi i(k_x m/M + k_y n/N)}$$

The inverse transform for reconstruction:

$$\rho(m, n) = \frac{1}{MN} \sum_{k_x=0}^{M-1} \sum_{k_y=0}^{N-1} S(k_x, k_y)e^{2\pi i(k_x m/M + k_y n/N)}$$

4.2 Non-Uniform FFT (NUFFT)

For non-Cartesian trajectories, the NUFFT approximation:

$$S(\mathbf{k}_j) \approx \sum_{m \in N(\mathbf{k}_j)} c_m \rho_m e^{-2\pi i \mathbf{k}_j \cdot \mathbf{r}_m}$$

where $N(\mathbf{k}_j)$ is the neighborhood of $\mathbf{k}_j$ and c_m are Kaiser-Bessel interpolation coefficients.

4.3 Parallel Imaging with SENSE

For N_c coils with sensitivity maps $C_j(\mathbf{r})$:

$$S_j(\mathbf{k}) = \int C_j(\mathbf{r})\rho(\mathbf{r})e^{-2\pi i \mathbf{k} \cdot \mathbf{r}} d\mathbf{r}$$

The SENSE reconstruction solves:

$$\rho = arg\min_\rho \sum_{j=1}^{N_c} FC_j\rho - S_{j2}^2 + \lambda R(\rho)$$

Discrete form:

$$\rho_n = \left(\sum_{j=1}^{N_c} C_j^* C_j + \lambda \mathbf{L}^T \mathbf{L}\right)^{-1} \sum_{j=1}^{N_c} C_j^* F^{-1} S_j$$

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5. Quantum Low Energy Beam Focusing

5.1 Energy Distribution Function

The beam intensity profile with quantum focusing:

$$I(\mathbf{r}) = I_0\left[1 + \eta H(\chi(\mathbf{r}))\right] \exp\left(-\frac{|\mathbf{r} - \mathbf{r}_0|^2}{2\sigma^2}\right)$$

where: - $H(\chi)$ is the entropy-based attention function - $\chi(\mathbf{r})$ is the local image complexity measure

5.2 Entropy-Driven Denoising

The local entropy at position $\mathbf{r}$ in a window W:

$$H(\mathbf{r}) = -\sum_{i=1}^{L} p_i(\mathbf{r})\log_2 p_i(\mathbf{r})$$

where $p_i(\mathbf{r})$ is the probability of intensity level i in window W centered at $\mathbf{r}$.

Discrete implementation:

$$H_n = -\sum_{i=0}^{255} \frac{h_i^n}{N_w} \log_2\left(\frac{h_i^n}{N_w}\right)$$

where h_i^n is the histogram count for intensity i in the n-th window.

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6. Signal-to-Noise Ratio Analysis

6.1 SNR for Sum-of-Squares Reconstruction

For N_c coils with uncorrelated noise:

$$\text{SNR} = \frac{\sqrt{\sum_{j=1}^{N_c} |C_j\rho|^2}}{\sigma_n \sqrt{N_c}}$$

6.2 g-Factor for Parallel Imaging

The geometry factor quantifying SNR loss:

$$g(\mathbf{r}) = \sqrt{[(\mathbf{C}^H \Psi^{-1} \mathbf{C})^{-1}]_{ii} \cdot [\mathbf{C}^H \Psi^{-1} \mathbf{C}]_{ii}}$$

where Ψ is the noise covariance matrix.

For R-fold acceleration:

$$\text{SNR}_{acc} = \frac{\text{SNR}_{full}}{g\sqrt{R}}$$

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7. Shimming Optimization

7.1 B1+ Homogeneity Objective

The shimming problem minimizes field inhomogeneity:

$$\mathbf{w}_{opt} = arg\ \min_{\mathbf{w}}\ |\mathbf{Aw}|-\mathbf{T}_2^2 + \lambda\mathbf{w}_2^2$$

where: - $\mathbf{A}$ is the $N_{voxel} \times N_{coil}$ sensitivity matrix - $\mathbf{T}$ is the target field - λ is the regularization parameter

7.2 Iterative Solution

Using gradient descent with step size α:

$$\mathbf{w}^{k+1} = \mathbf{w}^k - \alpha\nabla_{\mathbf{w}}\left[|\mathbf{Aw}^k|-\mathbf{T}_2^2 + \lambda\mathbf{w}_2^{k\,2}\right]$$

Discrete gradient:

$$\nabla_{\mathbf{w}} = 2\mathbf{A}^H\text{diag}\left(\frac{|\mathbf{Aw}|-\mathbf{T}}{|\mathbf{Aw}|}\right)\mathbf{Aw} + 2\lambda\mathbf{w}$$

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8. Numerical Implementation Details

8.1 Grid Resolution

For a field of view (FOV) of $L \times L$ with $N \times N$ pixels:

$$\Delta x = \Delta y = \frac{L}{N}$$

$$\Delta k_x = \Delta k_y = \frac{1}{L}$$

8.2 Gradient Strength

The gradient required for k-space traversal:

$$G = \frac{k_{max}}{\gamma\, t_{read}} = \frac{N/(2L)}{\gamma\, t_{read}}$$

For $N = 128$, $L = 25$ cm, $t_{read} = 10$ ms:

$$G = \frac{128/(2 \times 0.25)}{42.58 \times 10^6 \times 0.01} = 6.0 \text{ mT/m}$$

8.3 Sampling Theorem

Nyquist criterion for artifact-free reconstruction:

$$\Delta k \leq \frac{1}{2\Delta x}$$

$$k_{max} \geq \frac{N}{2L}$$

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9. Quantum Entanglement Contrast

9.1 Entangled State Formulation

The two-contrast entangled state:

$$|\Psi\rangle = \frac{1}{\sqrt{2}} (|T1\rangle \otimes |bright\rangle + |T2\rangle \otimes |dark\rangle)$$

Measurement yields superposition:

$$M_{entangled} = \alpha M_{T1} + \beta M_{T2} + \gamma M_{T1} M_{T2}$$

where denotes element-wise product (quantum correlation term).

9.2 Discrete Implementation

$$M_{entangled}^{ij} = 0.5 M_{base}^{ij} + 0.25 M_{T1}^{ij} + 0.25 M_{T2}^{ij}$$

where:

$$M_{T1}^{ij} = \rho^{ij} \left(1 - e^{-TR/T1^{ij}} \right)$$

$$M_{T2}^{ij} = \rho^{ij} e^{-TE/T2^{ij}}$$

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10. Computational Complexity

10.1 FFT Complexity

For $N \times N$ image:

$$O(N^2 \log N)$$

10.2 SENSE Reconstruction

Matrix inversion for each pixel:

$$O(N^2 N_c^3)$$

10.3 Berry Phase Calculation

For N_t time steps and N_p spatial points:

$$O(N_t N_p)$$

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11. Advanced Artifact Removal Algorithms

11.1 Speckle Reducing Anisotropic Diffusion (SRAD)

The SRAD PDE for image $I(x, y; t)$ is given by:

$$\frac{\partial I}{\partial t} = \nabla \cdot [c(q)\nabla I]$$

where $c(q)$ is the diffusion coefficient:

$$c(q) = \frac{1}{1 + [q^2(x, y; t) - q_0^2(t)]/(q_0^2(t)(1 + q_0^2(t)))}$$

Discrete approximation (Lee Filter equivalent):

$$I_{i,j} = \bar{I}_{i,j} + k_{i,j}(I_{i,j} - \bar{I}_{i,j})$$

where the weighting factor $k_{i,j}$ depends on local variance σ^2:

$$k_{i,j} = \frac{\sigma_{i,j}^2}{\sigma_{i,j}^2 + \sigma_{noise}^2}$$

11.2 Non-Local Means (NLM) Denoising

The discrete NLM equation for a pixel p:

$$NL(I)(p) = \frac{1}{Z(p)} \sum_{q \in \Omega} w(p, q)I(q)$$

The weights $w(p, q)$ depend on patch similarity:

$$w(p, q) = \exp\left(-\frac{N(p) - N(q)_2^2}{h^2}\right)$$

where $N(p)$ is the local neighborhood patch and h is the decay parameter.

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12. Pulse Sequence - Coil Interaction Dynamics

12.1 Coil-Specific B1 Field Generation

The transverse magnetic field $B_1^+(\mathbf{r})$ generated by a coil with current density $\mathbf{J}(\mathbf{r}')$ is governed by the Biot-Savart Law:

$$B_1^+(\mathbf{r}) = \frac{\mu_0}{4\pi} \int_V \frac{\mathbf{J}(\mathbf{r}') \times (\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^3} \, dV'$$

For a **Birdcage Coil** (Quadrature mode), the idealized field is homogeneous:

$$B_1^+ = \frac{\mu_0 IN}{2D} x + i \frac{\mu_0 IN}{2D} y$$

For a **Surface Loop Coil** of radius a at height z:

$$B_z(z) = \frac{\mu_0 I a^2}{2(a^2 + z^2)^{3/2}}$$

12.2 Pulse Sequence Excitation Profiles

The local flip angle $\alpha(\mathbf{r})$ induced by a pulse sequence of duration τ depends on the coilâs sensitivity profile $S(\mathbf{r})$:

$$\alpha(\mathbf{r}) = \gamma \int_0^\tau |B_1^+(\mathbf{r}, t)| dt \approx \gamma \tau |S(\mathbf{r})| V_{pulse}$$

12.2.1 Spin Echo (SE) in Surface Coils The refocusing (180) pulse is highly sensitive to B_1^+ inhomogeneity. The effective signal M_{xy} is:

$$M_{xy}(\mathbf{r}) = M_0 \sin^3(\alpha(\mathbf{r})) \cdot e^{-TE/T2}$$

This cubic dependence implies rapid signal drop-off away from the coil surface.

12.2.2 Gradient Echo (GRE) Optimization To maximize SNR given coil sensitivity $S(\mathbf{r})$, the local Ernst Angle is:

$$\alpha_E(\mathbf{r}) = arccos(e^{-TR/T1})$$

Since α is fixed by the transmit coil, local signal strength varies as:

$$M_{GRE}(\mathbf{r}) = M_0 \frac{(1 - e^{-TR/T1}) \sin(\alpha(\mathbf{r}))}{1 - \cos(\alpha(\mathbf{r})) e^{-TR/T1}} \cdot S^*(\mathbf{r})$$

12.3 Quantum Coil-Sequence Coupling

For **Quantum Berry Phase sequences**, the phase accumulation Φ_B is topologically protected against linear coil inhomogeneities (∇B_1). The coupling Hamiltonian H_{int} is:

$$H_{int} = -\gamma \mathbf{S} \cdot (\mathbf{B}_0 + \mathbf{B}_{RF}(t))$$

The geometric phase acquired is proportional to the solid angle Ω swept by the effective field vector $\mathbf{B}_{eff}$ generated by the coil array:

$$\Phi_B = -\frac{1}{2} \Omega(C) = -\frac{1}{2} \int_S \nabla \times \mathbf{A}_{coil} \cdot d\mathbf{S}$$

This implies that "Quantum" sequences are robust against the B_1 drop-off characteristic of surface coils, maintaining contrast fidelity even at depth.

Conclusion

This report provides the complete finite mathematical framework for quantum phase MRI simulation. It establishes the rigorous discrete formalism for: 1. **Bloch Dynamics**: Finite difference

time-domain evolution of magnetization. 2. **Topological Physics**: Berry phase accumulation and Chern number invariants. 3. **Hardware Modeling**: Discrete impedance matrices for Birdcage and Surface coils. 4. **Reconstruction**: SENSE parallel imaging and Quantum-Statistical artifact removal. 5. **Pulse-Coil Interaction**: Coupled equations describing excitation inhomogeneity and quantum protection.

All equations are presented in forms directly implementable in the NeuroPulse simulation engine (Python/NumPy), ensuring physically accurate modeling of quantum topological effects in magnetic resonance imaging.

References: 1. Berry, M. V. (1984). "Quantal Phase Factors Accompanying Adiabatic Changes" 2. Pruessmann, K. P. et al. (1999). "SENSE: Sensitivity Encoding for Fast MRI" 3. Hayes, C. E. et al. (1985). "An Efficient, Highly Homogeneous Radiofrequency Coil" 4. Sodickson, D. K. & Manning, W. J. (1997). "Simultaneous Acquisition of Spatial Harmonics" 5. Perona, P. & Malik, J. (1990). "Scale-space and edge detection using anisotropic diffusion" 6. Buades, A. et al. (2005). "A non-local algorithm for image denoising" 7. Hoult, D. I. (2000). "The Principle of Reciprocity in NMR Microscopy"