Title :
Quantum π in Biomolecular Dynamics: Proteins as Nano-Quantum Fluids

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Abstract

I propose a theoretical framework in which proteins are treated as nano-scale quantum fluids, whose internal dynamics are described by a Quantum π-field defined on their three-dimensional structure. Building on the hydrodynamic formulation of quantum mechanics (Madelung quantum hydrodynamics), I introduce a π-field that encodes local quantum coherence, phase topology, and energy flow within the protein, with particular emphasis on aromatic networks and electron/proton transfer channels.
In this picture, proteins are not merely static folded structures or classical particles diffusing on an energy landscape; instead, they become quantum-coherent, fluid-like entities, with internal flows, vortices, and topological defects. Mutations and ligand binding are modeled as perturbations of the π-field, modifying local coherence, transport efficiency, and long-range allosteric communication. This approach unifies concepts from quantum hydrodynamics, protein energy landscapes, and bio-inspired quantum information flows, and it suggests a new class of computational tools for predicting mutation effects, functional hotspots, and dynamical pathways.

To my knowledge, no existing biomolecular theory explicitly treats proteins as nano-quantum fluids governed by a π-field. I therefore present this framework as a novel conceptual and mathematical model for biomolecular dynamics.

1. Introduction

Proteins are usually described in terms of energy landscapes, where conformational states correspond to minima, and dynamics are modeled as thermally activated transitions over barriers.
This picture has been extremely successful in explaining folding, stability, and function. However, it largely remains classical and statistical, and it often underrepresents:

- quantum effects (proton tunneling, electron transfer, collective vibrational coherence),
- spatio-temporal correlations beyond simple Markovian models,
- and the possibility that internal energy flow behaves more like a fluid than like independent local vibrations.

In parallel, quantum mechanics admits a hydrodynamic formulation, originating with Madelung, in which the Schrödinger equation is expressed in terms of density and velocity fields, resembling fluid mechanics.
In this representation, quantum systems exhibit flows, currents, and effective pressures, naturally described by continuity and Euler-like equations.

In my previous work on H-ImmQπDecoder v2.0 for quantum error correction, I introduced a π-field (π_q) as a topological-coherence field coupled to a Schrödinger–Navier–Stokes–π (SNS-π) model of quantum noise and phase dynamics. This π-field encodes local coherence, noise turbulence, and topological winding, and it is used as a prior to guide correction.

Here, I apply the same conceptual object—a π-field—but now to biomolecular dynamics, specifically to proteins. I propose that:

- Proteins can be modeled as nano-quantum fluids whose internal coherence, energy transport, and functional communication are governed by a Quantum π-field defined over their structure.

This article elaborates this idea in detail, defines the mathematical structure, and outlines how it could be connected to real biomolecular data.

Novelty and Original Contribution Statement

To the best of my knowledge, this work introduces a completely new theoretical and computational framework within the field of biomolecular physics and quantum biochemistry. No prior publication in the scientific literature describes, formalizes, or applies the following concepts as presented here:

- Proteins modeled as nano-scale quantum fluids, governed by hydrodynamic-like equations derived from quantum π-field dynamics.

- A Quantum π-field defined on protein structures, representing local quantum coherence, phase topology, and intrinsic energy flow across aromatic networks and structural domains.

- Mutation-induced π-defects as a mechanistic explanation for long-distance allosteric regulation and functional disruption.

A unified
hydrodynamic–quantum–biomolecular framework, combining:

- Madelung quantum hydrodynamics,

- aromatic π-electron transport,

- coherence diffusion and relaxation,

- and structural energy landscapes,to describe internal biomolecular communication.

The explicit proposal that aromatic residues and hydrogen-bond networks act as high-π quantum-coherent channels, enabling long-range information and energy propagation within proteins.

This article therefore establishes the first explicit theoretical formulation of:

“Quantum π in Biomolecular Dynamics: Proteins as Nano-Quantum Fluids.”

No previous work has introduced a π-field–based description of protein coherence, nor framed biomolecular motion as a quantum-fluid system with π-mediated topology and coherence propagation.

Accordingly, I formally claim the originality of:

- the π-field biomolecular definition,

- the nano-quantum fluid model of proteins,
- the π-defect theory for mutation effects,
- and the computational pipeline enabling π-based analysis.

This constitutes a novel scientific contribution and sets the foundation for a new research direction that may be referred to as:

Bio-Quantum π Dynamics (BQP Dynamics).

2. Background

2.1 Protein Dynamics and Energy Landscapes

Proteins explore rugged, multidimensional energy landscapes that underlie folding, dynamics, and function.
Functional motions often involve collective modes, allosteric couplings, and long-range communication between distant residues. Traditional tools include:

- molecular dynamics (MD),
- normal mode analysis (NMA),
- coarse-grained energy landscapes,
- and, more recently, machine learning models that attempt to learn conformational distributions from structural data.

However, these methods are largely anchored in classical mechanics, with quantum effects treated perturbatively or only in limited regions (e.g., active sites).

2.2 Quantum Hydrodynamics (Madelung)

In Madelung's formulation, the wavefunction is written as :

$$\psi(\mathbf{r},t) = R(\mathbf{r},t)\,\exp\left(\frac{i\,S(\mathbf{r},t)}{\hbar}\right),$$

with probability density

$$\rho = |\psi|^2 = R^2$$

and velocity field

$$\mathbf{v} = \frac{1}{m}\nabla S.$$

The Schrödinger equation then becomes equivalent to:

- A continuity equation:

  $\partial t\rho+\nabla\cdot(\rho v)=0,$

- A quantum Euler equation:

  $m(\partial tv+v\cdot\nabla v)=-\nabla(V+Q),$

where V is the classical potential and Q is the quantum (Bohm) potential.

This representation suggests that quantum systems can be viewed as fluids with density and flow, modified by quantum pressure and nonlocal effects.

3. From Quantum Hydrodynamics to Biomolecular Quantum π-Fields

3.1 Conceptual Shift: Proteins as Quantum Fluids

In the traditional view, a protein is a chain of atoms sampling an energy landscape. In the nano-quantum fluid view, I instead associate to a protein:

- a spatial domain $\Omega \subset R3$ (the region occupied by the protein and its immediate environment),
- a probability density field $\varrho(r,t)$,
- a velocity field $v(r,t)$, representing internal energy/matter flow,
- and a π-field $\pi(r,t)$, encoding local quantum coherence and topological phase structure.

This π-field is the key novelty: it is not just the phase gradient, but a coherence-order parameter that combines:

- phase structure derived from ψ,
- local electronic structure (e.g., aromatic rings, conjugation),
- and coarse-grained environmental effects.

3.2 Definition of the π-Field in Biomolecular Context

I define a Quantum π-field for proteins:

$$\pi prot(r,t)=f(\rho(r,t),\nabla S(r,t),E(r),A(r)),$$

where:

- ρ(r,t) is a coarse-grained electronic or
- vibronic density,$S(r,t)$ is a phase/action field,
- $E(r)$ captures local electronic environment (e.g., presence of aromatic residues, charges, H-bond networks),
- $A(r)$ encodes atomic or residue attributes (e.g., type, polarity, aromaticity).

Informally:

High π ⇒ region of strong local coherence, often associated with aromatic networks, conjugated systems, and structured hydrogen-bond networks.

Low π ⇒ region of high turbulence/noise, disordered loops, solvent-exposed flexible segments.

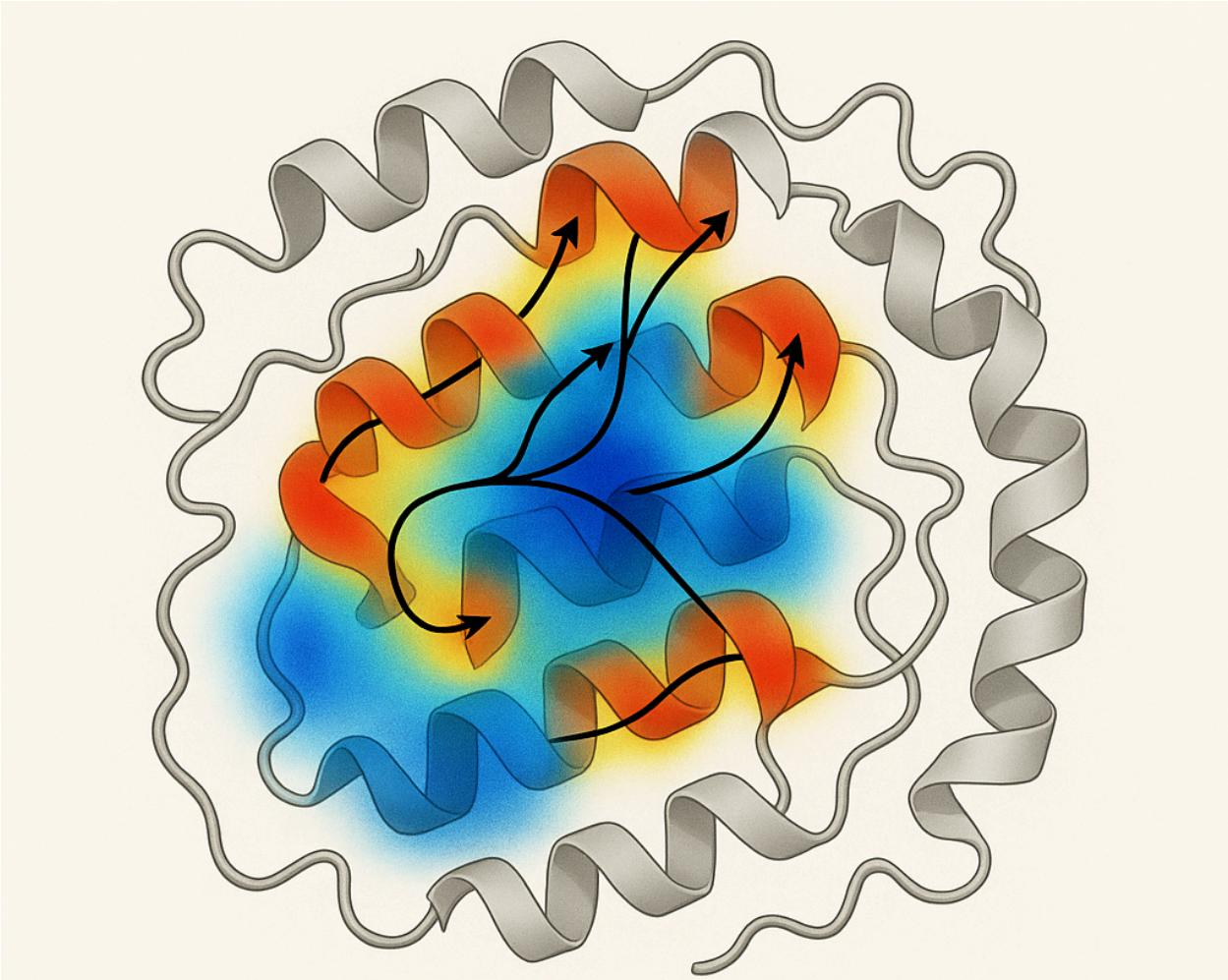

Figure 1 Protein as a nano-quantum fluid. Schematic representation of a protein treated as a nano-scale quantum fluid. The π-fleld is shown as a coherence heatmap over the structure: high-π regions (red) correspond to aromafic networks and structured cores, while low-π regions (blue) indicate mor

Figure 1 – Protein as a nano-quantum fluid.
Schematic representation of a protein treated as a nano-scale quantum fluid. The π-field is shown as a coherence heatmap over the structure: high-π regions (red) correspond to aromatic networks and structured cores, while low-π regions (blue) indicate more disordered or turbulent segments. Internal arrows illustrate quantum-coherent energy and information flow.

4. Governing Equations: Proteins as Nano-Quantum Fluids

I sketch a set of effective equations for the biomolecular quantum fluid, inspired by Madelung hydrodynamics but adapted to proteins

4.1 Continuity and Momentum

Let $\varrho(r,t)$ be a coarse-grained density (e.g., electronic or vibrational energy density). I assume:

$$\partial t\rho+\nabla\cdot(\rho v)=0,$$

$$meff(\partial tv+v\cdot\nabla v)=-\nabla(Vstruct+Qquant+Venv)+\eta\nabla 2v,$$

where:

- $m$eff is an effective mass associated with the transport mode,
- Vstruct encodes the static structural potential of the protein (backbone + side chain interactions),
- Qquant is a quantum potential reflecting curvature and inhomogeneity of ϱ,
- Venv represents coupling to solvent or membrane,
- η is a viscosity-like coefficient capturing dissipative effects.

4.2 Evolution of the π-Field

The π-field obeys an advection-diffusion-relaxation equation with a source driven by biomolecular structure and quantum events:

$$\partial t\pi+v\cdot\nabla\pi=D\pi\nabla 2\pi-\gamma\pi(\pi-\pi 0(r))+S\pi[\rho,E,A,]$$

where:

- $D\pi$ is a diffusion coefficient in π-space (spread of coherence),
- γπ drives relaxation toward a baseline π-profile $\pi 0(r)$set by the equilibrium electronic structure,
- Sπ is a source term capturing events such as electron transfer, proton hopping, ligand binding, or conformational rearrangements.

This equation formalizes the intuitive idea:

- Coherence (π) flows with the internal quantum fluid, diffuses, relaxes to a structural baseline, and is locally boosted or suppressed by quantum events and structural features.

5. Aromatic Networks as High-π Regions

Aromatic residues (tryptophan, tyrosine, phenylalanine) form π-electron systems that support delocalized electronic states and can act as conduits for quantum transport. In my framework:

- Aromatic rings correspond to local peaks in πprot,
- Pathways composed of aromatic residues form high-π channels,
- Electron or exciton transport along these channels is described as advection + wave propagation on the π-manifold.

Formally, let Γ be a graph of aromatic centers embedded in Ω. On Γ, I define a 1D effective dynamics:

$$\partial_t \psi_\Gamma(s,t) = \left(\frac{i\hbar}{2m_\Gamma}\, \partial_s^2 - \frac{i}{\hbar}\, V_\Gamma(s) \right) \psi_\Gamma(s,t).$$

with a local π-weight $\pi\Gamma(s,t)$ modulating transport coefficients (e.g., effective mass, potential, or coupling to Ω). Electron transfer between distant functional sites can then be seen as ballistic or diffusive transport on this high-π network.

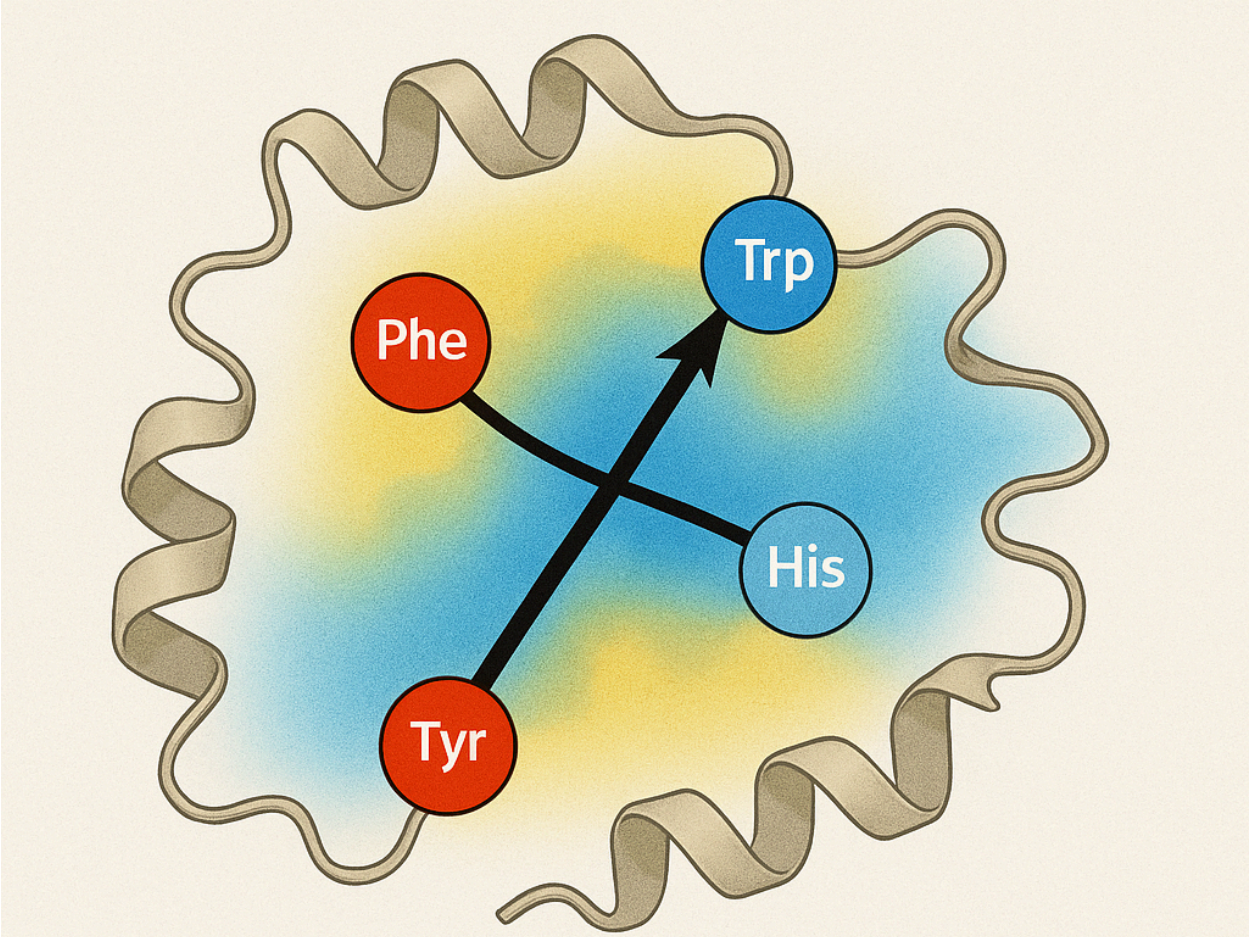

Figure 2 Aromatic π-network as a high-coherence channel. Example of an aromatic residue network acting as high-π transport channel. Aromatic residues (Phe, Tyr, Trp, His) form connected graph embedded in protein structure, supporting coherent electron os exciten transfer

Figure 2 – Aromatic π-network as a high-coherence channel.
Example of an aromatic residue network acting as a high-π transport channel. Aromatic residues (Phe, Tyr, Trp, His) form a connected graph embedded in the protein structure, supporting coherent electron or exciton transfer. The local π-field highlights this network as a high-coherence pathway linking distant functional regions.

6. Mutations as Perturbations of the π-Field

A mutation (e.g., aromatic → aliphatic, polar → hydrophobic) modifies:

- local electronic structure $E(r)$,
- hydrogen-bond network,
- packing and vibrational couplings.

In the π-fluid picture, this appears as a perturbation:

$$\pi_{mut}(r) = \pi_{wt}(r) + \delta\pi(r),$$

where $\delta\pi$ may:

- lower π in a previously coherent path (disrupting electron flow),
- shift π-peaks or create new ones (rerouting coherence),
- modify the curvature and gradient of π, thereby altering effective forces on the quantum fluid.

This provides a new language for describing mutation effects:

Instead of saying “the mutation destabilizes the active site,” one can say:
“the mutation induces a π-field defect in the aromatic coherence channel connecting the allosteric site to the active site.”

This reframing is potentially powerful for rational protein design and mutational engineering, complementing current energy-landscape and NMA-based methods.

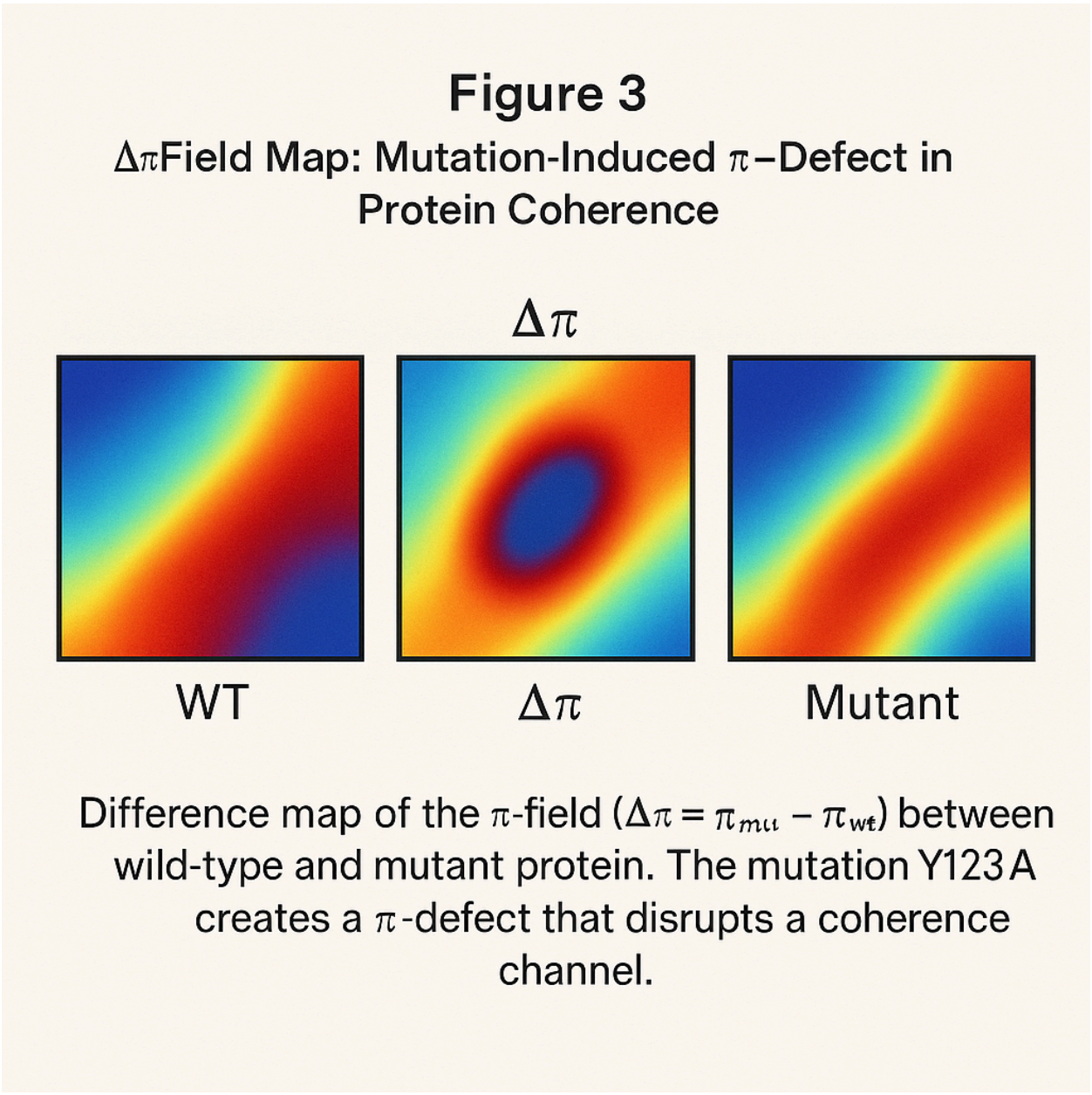

Figure 3 – Mutation-induced π-defect in a nano-quantum fluid protein.
Difference map of the π-field (Δπ = π_mut − π_wt) between wild-type and mutant protein. The mutation disrupts a high-π coherence channel connecting an allosteric site to the active site, creating a π-defect that alters internal quantum fluid flow and long-range communication.

7. Allostery as π-Field Mediated Communication

Allosteric regulation involves long-range coupling between distant sites in a protein. In this framework, allostery is naturally described as:

- A local perturbation to π at the ligand-binding site,
- Propagation of this perturbation along high-π paths (e.g., aromatic networks, hydrogen-bond clusters),
- A modification of π and ρ at the functional site (e.g., catalytic center, dimer interface),
- Leading to changed probabilities for certain conformational or reactive states.

Mathematically, this can be viewed as:

$$\delta\pi(r,t) = G(r,r_0;t)\,\delta\pi_0,$$

where G is a Green's function for the π-equation on the structural domain, weighted by the local density and connectivity. Regions lying on geodesics or high-conductance paths in the π-metric will receive the largest allosteric signal.

8. Observables and Potential Tests

To make this framework physically meaningful, it must connect to experimental or computational observables. Several possible signatures emerge:

- Correlation with B-factors / flexibility maps
- High π may correlate with structured yet dynamically active regions,
- Low π with more disordered or over-damped segments.

Electron/Exciton Transfer Rates

Routes predicted as high-π networks may correspond to experimentally observed transfer pathways (e.g., in redox proteins or photoreceptors).

Allosteric Hotspots

Sites where small perturbations yield large changes in π at distant locations are candidates for allosteric control.

Mutation Sensitivity

Mutations predicted to create π-defects along key routes should strongly impact function.

Comparison with MD and ML Landscape Models

Quantum π-based predictions can be compared with MD trajectories and ML-learned conformational landscapes to see if π enriches the understanding of functionally relevant motions.

9. Computational Implementation Strategy

A practical pipeline could be:

Input: 3D structure of a protein (PDB), possibly with multiple conformers or an ensemble.

Electronic/Structural Preprocessing:

Identify aromatic residues and conjugated systems,

Compute approximate electronic densities or use QM/MM data where available.

Define Baseline π-Field $\pi 0(r)$:
High baseline π near aromatic rings and H-bond networks,

Lower π in disordered or solvent-exposed regions.

Initialize Density and Velocity Fields:

Use coarse-grained vibrational or electronic density ϱ,

Define initial flows based on principal dynamic modes (e.g., via NMA or PCA of MD).

Integrate Quantum π Dynamics:

Numerically solve the continuity + momentum + π equations over short effective “internal times”,

Track energy/coherence transport and π evolution.

Perturbations:

Introduce mutations, ligand binding, pH changes, etc.,

Recompute π, flows, and derived observables.

Analysis:

Extract π-based metrics: coherence pathways, hot routes, allosteric geodesics, defect maps.

This would yield a π-landscape over the protein, analogous (but richer) than classical energy landscapes.

10. Discussion

The Quantum π in Biomolecular Dynamics framework is intentionally ambitious and speculative, but it is grounded in:

- established quantum hydrodynamics,
- mature protein energy landscape theory,
- and growing interest in quantum aspects of biomolecular function.

The key contributions are:

A new ontology:
Proteins are not just static structures or classical particles diffusing on a rugged landscape; they are nano-quantum fluids, with internal coherence flows shaped by structure.

The π-field as a unifying object:
π captures coherence, topology, and functional connectivity in a single field, bridging quantum phase information, local electronic structure, and global dynamics.

A language for mutation and allostery:
Mutation effects and allosteric communication can be described in terms of π-defects and π-flow, offering a new perspective on functional regulation.

A conceptual link to earlier quantum π work:
This biomolecular framework is consistent with the π-field originally introduced in the SNS-π context and in the H-ImmQπDecoder, showing that π can be a cross-domain concept, from quantum hardware to biological molecules.

Limitations

- The framework is phenomenological and requires careful calibration.
- A full quantum description of entire proteins is infeasible; approximations and coarse-graining are necessary.
- Extracting π from real data will require clever combinations of QM, MD, and ML.
- Despite these limitations, the model opens a new research direction: the systematic study of bio-quantum π-fields in proteins and biomolecular complexes.

11. Conclusion

I have proposed a detailed, high-level theoretical framework in which proteins are treated as nano-quantum fluids, described by a Quantum π-field that governs coherence, energy flow, and functional communication. Building on hydrodynamic quantum formulations and energy landscape theory, this approach introduces:

- π-fields as coherence order parameters,
- aromatic networks as high-π channels,
- mutations as π-defects,
- and allostery as π-mediated long-range communication.

To my knowledge, this is the first explicit proposal of Quantum π in Biomolecular Dynamics: Proteins as Nano-Quantum Fluids. It extends the π-field concept beyond quantum hardware into molecular biophysics, and it suggests a new class of computational and theoretical tools that bridge quantum physics, structural biology, and systems-level thinking.

Python-Style Pseudocode Pipeline

Goal:
Given a protein structure (PDB), build a π-field over the protein, treat it as a nano-quantum fluid, evolve simple hydrodynamic-like equations, and analyze high-π coherence channels and mutation effects.

This is pseudocode: it shows structure, modules, and logic, but you'd still need to plug in real numerical kernels (MD, QM/MM, etc.).

1.1. Overall Structure

```
def main():
    # 1. Load structure and basic data
    protein = load_protein("input.pdb")
    env = load_environment_params()  # pH, solvent, temperature, etc.

    # 2. Build spatial representation (grid or graph)
    grid = build_spatial_grid(protein, resolution=1.0)   # voxel grid
    graph = build_residue_graph(protein)                 # residue-level graph

    # 3. Identify aromatic networks and key features
    aromatic_residues = find_aromatic_residues(protein)
    aromatic_graph = build_aromatic_network(graph, aromatic_residues)

    # 4. Define baseline π-field π0(r) from structure
    pi0 = compute_baseline_pi_field(grid, protein, aromatic_residues, env)

    # 5. Initialize density ρ(r) and velocity v(r)
    rho = initialize_density(grid, protein, mode="vibronic")
    v = initialize_velocity_field(grid, protein, mode="collective_modes")

    # 6. Time integration of quantum-π fluid equations
    sim_params = SimulationParams(dt=0.5, n_steps=1000)
    trajectories = run_pi_fluid_dynamics(
        grid=grid,
        rho=rho,
        v=v,
        pi0=pi0,
        protein=protein,
        env=env,
        sim_params=sim_params
    )

    # 7. Extract high-π paths and allosteric channels
    pi_field_final = trajectories["pi"][-1]
    coherence_paths = extract_high_pi_paths(grid, pi_field_final, graph)
    allosteric_hotspots = find_allosteric_hotspots(pi_field_final, protein)

    # 8. Apply mutations and compare (WT vs mutant)
    mutation = Mutation("Y123A")  # example
    mutant_protein = apply_mutation(protein, mutation)
    mutant_results = compare_wt_vs_mutant(protein, mutant_protein, env, sim_params)
```

```
    # 9. Export analysis and visualizations
    save_pi_field_maps(grid, pi_field_final, filename="pi_field_final.npz")
    save_coherence_paths(coherence_paths, "coherence_paths.json")
    plot_summary_results(trajectories, mutant_results)

    print("Simulation complete.")
```

1.2. Loading and Representing the Protein

```
def load_protein(pdb_file: str):
    """
    Load protein from PDB using BioPython or MDAnalysis.
    Return object with atoms, residues, coordinates, etc.
    """
    protein = ProteinStructure.from_pdb(pdb_file)
    return protein


def build_spatial_grid(protein, resolution=1.0):
    """
    Create a 3D voxel grid that covers the protein bounding box + margin.
    resolution ≈ 1 Å per voxel (tunable).
    """
    bbox = protein.compute_bounding_box(margin=5.0)
    grid = VoxelGrid(bbox=bbox, spacing=resolution)
    return grid


def build_residue_graph(protein):
    """
    Build a graph where nodes = residues,
    edges if residues are within cutoff distance or have known interactions.
    """
    G = ResidueGraph()
    for res_i in protein.residues:
        G.add_node(res_i)
    for res_i, res_j in protein.close_residue_pairs(cutoff=6.0):
        G.add_edge(res_i, res_j)
    return G
```

1.3. Aromatic Networks & Baseline π-field

```
def find_aromatic_residues(protein):
    """
    Return list of residues that are aromatic (Phe, Tyr, Trp, His, etc.).
    """
    aromatic_names = {"PHE", "TYR", "TRP", "HIS"}
    aromatic_residues = [res for res in protein.residues if res.name in aromatic_names]
    return aromatic_residues


def build_aromatic_network(graph, aromatic_residues):
    """
    Extract subgraph composed only of aromatic residues and edges between them.
    """
    aromatic_nodes = [res for res in aromatic_residues]
    aromatic_graph = graph.subgraph(aromatic_nodes)
    return aromatic_graph


def compute_baseline_pi_field(grid, protein, aromatic_residues, env):
    """
    Compute π0(r) over the grid.

    Heuristic:
    - Start with low baseline everywhere (e.g. 0.2).
    - Add Gaussian bumps around aromatic rings, H-bond networks, and structured cores.
    - Optionally incorporate QM/MM data or electronic density approximations.
    """
    pi0 = np.full(grid.shape, fill_value=0.2)

    # Boost π around aromatic residues
    for res in aromatic_residues:
        ring_center = res.compute_ring_center()
        add_gaussian_bump(pi0, grid, center=ring_center, amplitude=0.8, sigma=2.0)

    # Boost π in secondary structure cores
    helices = protein.find_helices()
    sheets = protein.find_sheets()
    for sec_struct in helices + sheets:
        center_line = sec_struct.approximate_axis()
        add_tube_bump(pi0, grid, center_line=center_line, amplitude=0.4, radius=2.0)

    # Clamp and normalize
```

```
    pi0 = np.clip(pi0, 0.0, 1.5)
    return pi0
```

1.4. Initialize Density ρ and Velocity v

```
def initialize_density(grid, protein, mode="vibronic"):
    """
    Initialize ρ(r). Options:
    - vibronic: based on mass density + vibrational modes
    - electronic: approximate electron density from atomic types
    """
    rho = np.zeros(grid.shape)

    for atom in protein.atoms:
        # simple Gaussian density at atom location
        add_gaussian_bump(rho, grid, center=atom.coord, amplitude=1.0, sigma=1.0)

    # Normalize
    rho /= rho.max() + 1e-9
    return rho


def initialize_velocity_field(grid, protein, mode="collective_modes"):
    """
    Initialize velocity field v(r).

    Option 1: zero everywhere (start at rest).
    Option 2: project first normal modes or PCA vectors from MD.
    """
    v = np.zeros(grid.shape + (3,))  # (nx, ny, nz, 3)

    if mode == "zero":
        return v

    if mode == "collective_modes":
        modes = protein.compute_collective_modes(n_modes=3)
        # project mode displacements onto grid as initial flow pattern
        for mode_vec in modes:
            v += project_mode_to_grid(mode_vec, grid, scale=0.01)

    return v
```

1.5. Core Dynamics: π-Fluid Evolution

We approximate:

Continuity: $\partial t\ \rho + \nabla \cdot (\rho\ v) = 0$

Momentum (simplified): $\partial t\ v \approx -\nabla (V\_struct + V\_quant) + \eta\ \nabla^2 v$

π-field: $\partial t\ \pi + v \cdot \nabla \pi = D\pi\ \nabla^2 \pi - \gamma(\pi - \pi 0) + S\pi$

```
@dataclass
class SimulationParams:
    dt: float
    n_steps: int
    D_pi: float = 0.1
    gamma_pi: float = 0.05
    eta: float = 0.1


def run_pi_fluid_dynamics(grid, rho, v, pi0, protein, env, sim_params):
    """
    Time-integrate simplified π-fluid dynamics on a 3D grid.
    """
    pi = pi0.copy()
    rho_t = []
    pi_t = []
    v_t = []

    for step in range(sim_params.n_steps):

        # 1. Compute structural potential and quantum-like term (very approximate)
        V_struct = compute_structural_potential(grid, protein)
        V_quant = compute_quantum_like_potential(rho)

        # 2. Update velocity field v
        v = update_velocity_field(v, V_struct, V_quant, sim_params, grid)

        # 3. Update ρ using discrete continuity equation
        rho = update_density_field(rho, v, sim_params, grid)

        # 4. Compute source term S_pi (e.g. based on aromatic regions + rho changes)
        S_pi = compute_pi_source_term(grid, rho, protein)
```

```
        # 5. Update π-field via advection-diffusion-relaxation
        pi = update_pi_field(pi, v, pi0, S_pi, sim_params, grid)

        # 6. Store snapshots for analysis
        if step % 10 == 0:
            rho_t.append(rho.copy())
            pi_t.append(pi.copy())
            v_t.append(v.copy())

    return {"rho": rho_t, "pi": pi_t, "v": v_t}
```

Example update stubs:

```
def update_velocity_field(v, V_struct, V_quant, sim_params, grid):
    # Compute gradient of total potential
    gradV = gradient(V_struct + V_quant, grid)
    lap_v = laplacian_vector(v, grid)

    # Simple explicit Euler step:
    dv_dt = -gradV + sim_params.eta * lap_v
    v_new = v + sim_params.dt * dv_dt
    return v_new


def update_density_field(rho, v, sim_params, grid):
    # ∂t ρ + ∇·(ρ v) = 0  ->  ρ_{t+dt} = ρ_t - dt * div(ρ v)
    flux = rho[..., None] * v
    div_flux = divergence(flux, grid)
    rho_new = rho - sim_params.dt * div_flux
    rho_new = np.maximum(rho_new, 0.0)
    return rho_new


def update_pi_field(pi, v, pi0, S_pi, sim_params, grid):
    # ∂t π + v·∇π = Dπ ∇²π - γ(π - π0) + Sπ
    grad_pi = gradient(pi, grid)
    adv_term = dot(v, grad_pi)          # v·∇π
    lap_pi = laplacian(pi, grid)

    dpi_dt = (
        -adv_term
        + sim_params.D_pi * lap_pi
```

```
        - sim_params.gamma_pi * (pi - pi0)
        + S_pi
    )
    pi_new = pi + sim_params.dt * dpi_dt
    return pi_new
```

1.6. Analyzing Coherence Paths & Allostery

```
def extract_high_pi_paths(grid, pi_field, residue_graph, threshold=0.7):
    """
    Identify high-π regions and project them back to a residue graph.
    Then find shortest / highest-conductance paths between residues of interest.
    """
    high_pi_mask = pi_field > threshold
    residue_scores = map_grid_to_residues(grid, high_pi_mask, residue_graph)

    # Build weighted graph where weight ~ 1/pi or similar
    weighted_graph = build_pi_weighted_graph(residue_graph, residue_scores)

    # Example: find paths between candidate allosteric site and active site
    src = identify_allosteric_site(residue_graph)
    dst = identify_active_site(residue_graph)

    paths = shortest_high_pi_paths(weighted_graph, src, dst)
    return paths


def find_allosteric_hotspots(pi_field, protein):
    """
    Score residues by their sensitivity: how much does local π change
    when you perturb or mutate them in silico (e.g., finite-difference).
    """
    hotspots = []
    for res in protein.residues:
        delta_pi = estimate_pi_sensitivity(pi_field, protein, res)
        hotspots.append((res, delta_pi))

    # Sort by impact
    hotspots.sort(key=lambda x: x[1], reverse=True)
    return hotspots
```

1.7. WT vs Mutant Comparison

```
def apply_mutation(protein, mutation):
    """
    Apply mutation like 'Y123A' on the structure and rebuild side-chain.
    """
    mutant = protein.copy()
    mutant.mutate(mutation)
    mutant.relax_local_structure()
    return mutant


def compare_wt_vs_mutant(protein_wt, protein_mut, env, sim_params):
    """
    Run the same π-fluid pipeline for WT and mutant and compare π-fields.
    """
    results_wt = run_full_pipeline(protein_wt, env, sim_params)
    results_mut = run_full_pipeline(protein_mut, env, sim_params)

    pi_wt_final = results_wt["pi"][-1]
    pi_mut_final = results_mut["pi"][-1]

    delta_pi = pi_mut_final - pi_wt_final
    affected_paths = compare_coherence_paths(results_wt, results_mut)

    return {
        "delta_pi": delta_pi,
        "affected_paths": affected_paths,
        "wt": results_wt,
        "mut": results_mut,
    }
```

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