MATHEMATICAL FOUNDATIONS OF QUANTUM MECHANICS

MATRIX MECHANICS

The Role of Matrices in Quantum Formulation

An axiomatic breakdown of how linear algebra translates physical reality into operators and states.

1. THE PARADIGM: PHYSICAL QUANTITIES AS MATRICES

In quantum theory, physical variables are not scalar functions. As formulated by Werner Heisenberg, observables are linear operators. When mapped to a discrete orthonormal basis $\{|n\rangle\}$, these operators become complex matrices.

Matrix Element Derivation: An operator A is represented by elements A_{mn} calculated via the inner product:

$$A_{mn} = \langle m| A |n\rangle \quad \Longrightarrow \quad A = \sum_{m,n} A_{mn} |m\rangle \langle n|$$

State vectors $|\psi\rangle$ map directly to single-column matrices: $[\psi]_n = \langle n|\psi\rangle$.

2. ESSENTIAL MATRIX CLASSES AND PHYSICAL INTERPRETATIONS

The physical laws of quantum mechanics constrain operators to strict algebraic properties:

- **Hermitian Matrices ($A^\dagger = A$):** Represent physical observables (Energy, Momentum, Spin). Their conjugate transpose leaves them invariant. This guarantees exclusively real eigenvalues (measurable traits) and orthogonal eigenvectors.
- **Unitary Matrices ($U^\dagger U = I$):** Represent closed-system time evolution and quantum logic gates. They preserve the inner product ($\langle U\psi|U\psi\rangle = \langle\psi|\psi\rangle$), ensuring total probability remains exactly 1.

3. MATRIX NON-COMMUTATIVITY & PHYSICAL UNCERTAINTY

Unlike classical numbers, matrix multiplication depends on order ($AB \neq BA$). This algebraic property is the mathematical origin of the Heisenberg Uncertainty Principle.

The Commutator: Define $[A, B] = AB - BA$. If $[A, B] \neq 0$, the corresponding physical properties cannot be measured simultaneously with infinite precision.

Canonical Position-Momentum Commutator: $[X, P] = i\hbar I$

4. THE DENSITY MATRIX (ρ) & OPEN SYSTEMS

When a quantum system is entangled with an external environment or contains statistical uncertainties, it can no longer be written as a pure state vector $|\psi\rangle$. It must be modeled using a **Density Matrix**.

PROPERTIES OF THE DENSITY MATRIX

For a statistical ensemble of states $|\psi\rangle_i$ distributed with probabilities p_i:

$$\rho = \sum_i p_i |\psi_i\rangle \langle\psi_i| \quad \Longrightarrow \quad \text{Conditions: } \mathrm{Tr}(\rho) = 1, \quad \rho^\dagger = \rho, \quad \rho \geq 0$$

Pure vs Mixed Test: $\mathrm{Tr}(\rho^2) = 1$ implies a pure state, while $\mathrm{Tr}(\rho^2) < 1$ proves environmental decoherence.

5. DIMENSION SCALING VIA KRONECKER PRODUCTS

When independent quantum systems combine, their matrix dimensions scale exponentially via the **Kronecker (Tensor) Product** $\otimes$. If two single-qubit gates are executed in parallel, their global matrix transformation is represented by:

$$A \otimes B = \begin{pmatrix} A_{11}B & A_{12}B \\ A_{21}B & A_{22}B \end{pmatrix} \quad \Longrightarrow \quad \text{Scales space from 2 dimensions to } 2^N$$