

Introduction

As seen from Equation (1.1), a quantum system is characterized by the system's Hamiltonian, which is the key part of Schrödinger's equation that determines how the wave function evolves in time. The resulting time development is a deterministic *unitary* evolution and it has very particular characteristics. The Hamiltonian represents the energies of the system and its interactions and the unitary evolution is determined by these energies.

The unitary operator U corresponding to the Hamiltonian is just given by:

$$U(t) = \exp(-iHt/\hbar). \quad (2.1)$$

As discussed further in the theoretical development, Equation (2.1) is a result of *Stone's Theorem* [11], and the form of U can also be related to any symmetries that the system possesses (e.g., if the system doesn't change by rotations or translations in space) by *Wigner's Theorem* [12]. Quantum theory depicts the states of the world as evolving linearly according to a unitary operator U so that the state at a time t is given by:

$$|\psi(t)\rangle = U|\psi(0)\rangle. \quad (2.2)$$

These states are probability amplitudes made up of a space of complex unit vectors $|\psi\rangle$ (called a *Hilbert space*, a complete vector space with an inner product). Such states $|\psi\rangle$ in Hilbert space are also referred to as pure states. The imaginary number i in Equation (2.1) alerts us that quantum mechanics requires complex numbers in contrast to classical mechanics.

There can exist additional quantum states of nature that are outside the class of pure states. Quantum theory developed by von Neumann [13] included this generalization of pure states to include the set of *mixed states* [14, p. 100]. A mixed state has no representation in the set of pure states $|\psi\rangle$ in the representative Hilbert space and one must resort to the extension of pure states to the set of density matrices. A pure state $|\psi\rangle$ can also be represented by a density matrix defined by $\rho \equiv |\psi\rangle\langle\psi|$. A mixed state is a positive density matrix for which $\text{Tr}(\rho^2) < 1$, whereas for a pure state $\text{Tr}(\rho^2) = 1$. Gleason's theorem [15] demonstrates that if the Hilbert space dimension is greater than 2, then the general expression for the expectation value of an operator A is: $\langle A \rangle = \text{tr}[A\rho]$, where ρ is the density operator. This implies that density operators are the most general description of quantum mechanical states.

The effect of a unitary operation does not depend on the state $|\psi\rangle$ to which it applies. This is a consequence of the linearity of the evolution. Quantum state unitary evolution is linear in wave function (in Chapter 7, we will also encounter quantum state evolution that is linear in density operator) because the operation satisfies:

$$U(a|\psi\rangle + b|\phi\rangle) = aU|\psi\rangle + bU|\phi\rangle. \quad (2.3)$$

This is the origin of the superposition principle in quantum mechanics, so that the linear superposition of two wave functions is also a legitimate wave function. As discussed in Chapter 1, the superposition principle in conjunction with Born's rule is the basis for understanding the double-slit experiments, [Figure 1.4](#).