Evolution in the Eigenstate Basis

An operator is unitary if its Hermitian conjugate $U^\dagger$ (found by taking the transpose and complex conjugate $U^\dagger \equiv (U^*)^T$) is equal to its inverse $U^\dagger = U^{-1}$, or

$$U^\dagger U = UU^\dagger = I \tag{2.6}$$

As a consequence, the eigenvalues of U have unit norm and take the form $\lambda_j = \exp(i\varphi_j)$. Note that if U is unitary, then so is $U^\dagger$. If U_1 and U_2 are unitaries, then so is the product $U = U_1U_2$. The invertibility of U implies that information is preserved during the evolution. Equation (2.6) implies that the inner product of states is preserved under unitary evolution, i.e., if $|\acute{\psi}\rangle = U|\psi\rangle$ and $|\acute{\varphi}\rangle = U|\varphi\rangle$, then $\langle\acute{\psi}|\acute{\varphi}\rangle = \langle\psi|U^\dagger U|\varphi\rangle = \langle\psi|\varphi\rangle$. In particular, this implies that the net probability of finding the particle (denoted by $p(t)$) is always preserved for all time under unitary evolution.

That is,

$$p(t) = \langle\psi(t)|\psi(t)\rangle = \langle\psi(0)|U^\dagger U|\psi(0)\rangle = \langle\psi(0)|\psi(0)\rangle = p(0). \tag{2.7}$$

Note that Equation (2.1) implies that $U^\dagger(t) = U(-t)$ so that the unitary operator $U^\dagger$ simply reverses the time evolution from U and thus it is a time-reversible transformation. We can also see that Equations (2.1) and (2.2) are equivalent to the time-dependent Schrödinger equation since

$$i\hbar\frac{\partial U|\psi(0)\rangle}{\partial t} = HU|\psi(0)\rangle$$

or

$$i\hbar\frac{\partial|\psi(t)\rangle}{\partial t} = H|\psi(t)\rangle. \tag{2.8}$$

This is the quantum mechanical equation that has long been considered relevant for *closed* or isolated systems. In the Heisenberg representation, the time-dependence is unitarily transferred from the wave function $|\psi(t)\rangle$ to the operators of the problem such as G, which obeys

$$\frac{dG}{dt} = -\frac{i}{\hbar}[G, H]. \tag{2.9}$$

In finite dimensions and when the Hamiltonian is time-independent, the time evolution unitary operator in Equation (2.1) can be decomposed into a series of simpler pieces (this is allowed by the *spectral theorem* [37, p. 221]) as:

$$U = \sum_k e^{iE_k t} |\phi_k\rangle\langle\phi_k| \tag{2.10}$$

for any time t. The spectral theorem in infinite dimensions becomes subtler and a rigorous operational description can be problematic [37]. This simplification happens by using new states called energy eigenstates $|\phi_k\rangle$ of the Hamiltonian which have the property $H|\phi_k\rangle = E_k|\phi_k\rangle$, and the constant E_k is called the energy eigenvalue. If the state of the system is written in this eigenstate basis

$$|\psi(t)\rangle = \sum_k a_k(t)|\phi_k\rangle \tag{2.11}$$

where $\sum_k |a_k(t)|^2 = 1$, then from Equations (2.8) and (2.11) we can conclude that (see Exercise 2.1 in the book or kindle version of theQMP)

$$a_k(t) = a_k(0)\exp(-iE_k t/\hbar). \tag{2.12}$$

The unitary evolution is determined by the total Hamiltonian which may describe several subsystems and their mutual interactions. If the subsystems are not interacting, then the total unitary operator is simply a product of unitary operators. For example, with two non-interacting subsystems A and B, the unitary operator of the total system would be a product of local unitary operators, $U_{AB} = U_A U_B$. In this case, the subsystems evolve independently and it would be possible to average over or *trace out* the degrees of freedom of system B and still have subsystem A described by a unitary evolution. However, even in the presence of interactions, there are cases where the tracing out of subsystem degrees of freedom can still leave the evolution of the remaining subsystems unitary but instead it becomes governed by a different *effective Hamiltonian* instead of the original Hamiltonian in Equation (2.1). For example, this can occur when the timescales of different subsystems are quite disparate and the technique of *adiabatic elimination* [38] [39] can be used to eliminate the fast degrees of freedom which are adiabatically following the evolution of the slow degrees of freedom. This results in an effective Hamiltonian H_{eff} which accurately describes the unitary evolution, $U_{eff} = \exp(-iH_{eff}\mathrm{t})$, of the remaining slow degrees of freedom in this adiabatic regime. In other cases, it may be possible to exploit symmetries in the Hamiltonian to enable construction of a special unitary transformation $\widetilde{U}$ to transform the system into an effective Hamiltonian, $H_{eff} = \widetilde{U}\, H \widetilde{U}^{\dagger}$. This is yet another role for unitary transformations in quantum mechanics and is once again due to the presence of symmetries. An example is given in Exercise 2.12 in the book or kindle version of theQMP. The quantum evolution for more general cases when there are interactions between the subsystems is discussed in a later section.