Quantum Time Evolution and Measurement [lam6]

Classical time evolution:

The time evolution of classical dynamical systems is expressed by differential equations for dynamical variables such as the following:

▷ Lagrange equations are second-order ODEs for generalized coordinates,

$$\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}_i} - \frac{\partial \mathcal{L}}{\partial q_i} = 0 \quad : \; i = 1, \ldots, n,$$

derived from a Lagrangian function $\mathcal{L}(q_1, \ldots, q_n; \dot{q}_1, \ldots, \dot{q}_n)$.

▷ Canonical equations are first-order ODEs for canonical coordinates,

$$\dot{q}_i = \frac{\partial \mathcal{H}}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial \mathcal{H}}{\partial q_i} \quad : \; i = 1, \ldots, n,$$

derived from a Hamiltonian function $\mathcal{H}(q_1, \ldots, q_n; p_1, \ldots, p_n)$.

▷ Hamilton's equations are first-order equations for a set of elementary variables for which an energy function and symplectic structure have been established:

- Elementary dynamical variables: $u_1, \ldots, u_m$.
- Energy function: $\bar{\mathcal{H}}(u_1, \ldots, u_m)$.
- Symplectic structure (set of elementary Poisson brackets):

$$\{u_i, u_j\} = B_{ij}(u_1, \ldots, u_m).$$

- Hamilton's equations: $\dot{u}_i = \{u_i, \bar{\mathcal{H}}\}$.

The time evolution of an arbitrary dynamical variable follows as it is constructed as a function of the $q_i, \dot{q}_i$ or q_i, p_i or u_i.

The time evolution is deterministic if the state of the system is specified as a set of initial conditions for the applicable variables.

Determinism in the classical time evolution is undermined by computational instabilities in nonintegrable i.e. chaotic systems:

- Mapping out the trajectory of a classical dynamical system over a given time interval and a given mesh size requires N bits of information.
- Computing the same trajectory with acceptable accuracy takes M bits of information.
- The N bits are used for encoding coordinates whereas the M bits are used for encoding the algorithm and the initial conditions.

- Determinacy of classical dynamics can be declared to hinge on whether the ratio M/N tends toward zero or a nonzero value as the time interval of the trajectory in question grows to infinity.
- Trajectories with nearby initial conditions tend to diverge no faster than some power of time in integrable systems but exponentially in time in nonintegrable systems.
- The difference is related to the fact that the phase space of an integrable system is foliated by invariant tori, which severely confine the course of trajectories. The foliation is partially destroyed in chaotic systems.
- The consequence is that we have $M = M_0 + a \ln t$ and $M = M_0 + bt$ for integrable and nonintegrable systems, respectively. M_0 reflects the information of the algorithm and a, b are constants. On the other hand we have $N \propto t$ for mapping out any kind of trajectory.
- Hence $M/N \to 0$ applies (in general) only to integrable systems. The time evolution is truly deterministic in the sense that the N bits used to map out the trajectory are unnecessary. The course of that trajectory is predictable by the much smaller number of M bits.
- In chaotic systems, on the other hand, M/N remains nonzero for long trajectories. The number of digits needed to specify the initial conditions with sufficient accuracy grows proportional to t. The N bits used to map out the trajectory are not made redundant by the algorithm.

Quantum time evolution:

In quantum mechanics, indeterminacy comes into play quite differently.

- The time evolution of state vectors or density operators is linear, thus free of the instabilities associated with nonlinear equations of motion that govern classical trajectories.
- The initial conditions classically encapsulated in a phase point are subject to the quantum indeterminacy $\Delta\mathrm{Q}\Delta\mathrm{P} \geq \frac{1}{2}\hbar$ discussed in [lam4].
- Irreducible quantum indeterminacy is manifest in expectation values and variances or covariances associated with observables represented by non-commuting operators.

In the following we briefly describe how the quantum time evolution is described as carried by state vectors, observables, or density operators.

Schrödinger equation:

The time evolution of a pure quantum state $|\psi(t)\rangle$ of a quantum system specified by Hamiltonian $\mathcal{H}$ is governed by the Schrödinger equation,

$$\imath\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \mathcal{H}|\psi(t)\rangle.$$

We consider an autonomous system $\mathcal{H}_0$ (e.g. an atom), which then experiences a time-dependent perturbation $\mathcal{V}(t)$ (e.g. an electromagnetic wave):

$$\mathcal{H}(t) = \mathcal{H}_0 + \mathcal{V}(t).$$

Eigenvalue equation: $\mathcal{H}_0|n\rangle = E_n|n\rangle \quad : \; n = 0, 1, 2, \ldots$

Non-stationary state: $|\psi(t)\rangle = c_n(t)|n\rangle$.

Time evolution under $\mathcal{H}_0$: $|\psi(t)\rangle = \sum_n c_n(0)e^{-\imath\omega_n t}|n\rangle$.

$$\imath\hbar\dot{c}_n|n\rangle = E_n|n\rangle \quad \Rightarrow \; c_n(t) = c_n(0)e^{-\imath\omega_n t}, \quad \hbar\omega_n = E_n.$$

Effect of $\mathcal{V}(t)$ on time evolution: the expansion coefficients become (more or less slowly) time-dependent: $c_n(0) \to \tilde{c}_n(t)$.

Ansatz: $|\psi(t)\rangle = \sum_n \tilde{c}_n(t)e^{-\imath\omega_n t}|n\rangle$.

Substitution into Schrödinger equation:

$$\imath\hbar\sum_n \dot{\tilde{c}}_n(t)e^{-\imath\omega_n t}|n\rangle + \underbrace{\imath\hbar\sum_n(-\imath\omega_n)\tilde{c}_n(t)e^{-\imath\omega_n t}|n\rangle}$$
$$= \overbrace{\sum_n(\hbar\omega_n)\tilde{c}_n(t)e^{-\imath\omega_n t}|n\rangle} + \sum_n \tilde{c}_n(t)e^{-\imath\omega_n t}\mathcal{V}(t)|n\rangle.$$

Multiply simplified equation with $\langle m|e^{\imath\omega_m t}$:

$$\imath\hbar\dot{\tilde{c}}_n(t) = \sum_{mn} e^{\imath(\omega_m-\omega_n)t}\langle m|\mathcal{V}(t)|n\rangle\tilde{c}_n(t).$$

Interaction representation: $\imath\frac{\partial}{\partial t}|\tilde{\psi}(t)\rangle = \tilde{\mathcal{V}}(t)|\tilde{\psi}(t)\rangle$,

$$|\tilde{\psi}(t)\rangle \doteq e^{\imath\mathcal{H}_0 t/\hbar}|\psi(t)\rangle = \sum_n \tilde{c}_n(t)|n\rangle, \quad \tilde{\mathcal{V}}(t) \doteq e^{\imath\mathcal{H}_0 t/\hbar}\mathcal{V}(t)e^{-\imath\mathcal{H}_0 t/\hbar}.$$

Coupled linear ODEs for expansion coefficients:

$$\Rightarrow \; \frac{d}{dt}\tilde{c}_n(t) = -\frac{\imath}{\hbar}\sum_{nm}\tilde{\mathcal{V}}_{nm}(t)\tilde{c}_m(t), \quad \tilde{\mathcal{V}}_{nm}(t) \doteq e^{\imath(\omega_n-\omega_m)t}\langle n|\mathcal{V}(t)|m\rangle.$$

Heisenberg equation:

Consider autonomous system with Hamiltonian $\mathcal{H}$.

Time evolution operator: $\mathcal{U}(t) \doteq e^{-\imath\mathcal{H}t/\hbar}$.

Unitarity: $\mathcal{U}^\dagger = e^{\imath\mathcal{H}t/\hbar} \quad \Rightarrow \; \mathcal{U}^\dagger\mathcal{U} = \mathcal{I}$.

Schrödinger equation: $\imath\hbar\dfrac{\partial}{\partial t}|\psi(t)\rangle = \mathcal{H}|\psi(t)\rangle$.

Formal solution: $|\psi(t)\rangle = \mathcal{U}(t)|\psi(0)\rangle$.

Expectation value of operator $\mathcal{A}$:

$$\langle\psi(t)|\mathcal{A}|\psi(t)\rangle = \langle\psi(0)|\mathcal{U}^\dagger(t)\mathcal{A}\mathcal{U}(t)|\psi(0)\rangle = \langle\psi(0)|\mathcal{A}(t)|\psi(0)\rangle.$$

– In the expression on the left, the time evolution is carried by the state and governed by the Schrödinger equation (above).

– In the expression on the right, the time evolution is carried by the observable and governed by the Heisenberg equation (below).

Time evolution of $\mathcal{A}$: $\mathcal{A}(t) = \mathcal{U}^\dagger(t)\mathcal{A}\mathcal{U}(t) = e^{\imath\mathcal{H}t/\hbar}\mathcal{A}e^{-\imath\mathcal{H}t/\hbar}$.

$$\Rightarrow \; \frac{d}{dt}\mathcal{A}(t) = \frac{d\mathcal{U}^\dagger}{dt}\mathcal{A}\mathcal{U} + \mathcal{U}^\dagger\mathcal{A}\frac{d\mathcal{U}}{dt}.$$

Use $\dfrac{d\mathcal{U}^\dagger}{dt} = \dfrac{\imath}{\hbar}\mathcal{U}^\dagger\mathcal{H}, \quad \dfrac{d\mathcal{U}}{dt} = -\dfrac{\imath}{\hbar}\mathcal{H}\mathcal{U}, \quad [\mathcal{H},\mathcal{U}] = [\mathcal{H},\mathcal{U}^\dagger] = 0.$

$$\Rightarrow \; \frac{d}{dt}\mathcal{A}(t) = \frac{\imath}{\hbar}\Big(\mathcal{U}^\dagger\mathcal{H}\mathcal{A}\mathcal{U} - \mathcal{U}^\dagger\mathcal{A}\mathcal{H}\mathcal{U}\Big) = \frac{\imath}{\hbar}\Big(\mathcal{H}\mathcal{U}^\dagger\mathcal{A}\mathcal{U} - \mathcal{U}^\dagger\mathcal{A}\mathcal{U}\mathcal{H}\Big).$$

Heisenberg equation: $\dfrac{d}{dt}\mathcal{A}(t) = \dfrac{\imath}{\hbar}[\mathcal{H}, \mathcal{A}(t)]$.

Von Neumann equation:

Mixed quantum state of autonomous system: $\rho = \sum_\psi |\psi\rangle\langle\psi|$.

Its time evolution can be constructed using the Schrödinger equation:

$$\frac{\partial\rho}{\partial t} = \sum_\psi\left(\frac{\partial|\psi\rangle}{\partial t}\langle\psi| + |\psi\rangle\frac{\partial\langle\psi|}{\partial t}\right) = -\frac{\imath}{\hbar}\sum_\psi\big(\mathcal{H}|\psi\rangle\langle\psi| - |\psi\rangle\langle\psi|\mathcal{H}\big).$$

Von Neumann equation: $\dfrac{\partial\rho}{\partial t} = -\dfrac{\imath}{\hbar}[\mathcal{H}, \rho] \quad$ (quantum Liouville equation).

Application to $\mathcal{H}(t) = \mathcal{H}_0 + \mathcal{V}(t)$ with $\mathcal{H}_0|n\rangle = \hbar\omega_n|n\rangle$:

Von Neumann equation: $\dfrac{\partial\rho}{\partial t} = -\dfrac{\imath}{\hbar}[\mathcal{H}_0, \rho] - \dfrac{\imath}{\hbar}[\mathcal{V}(t), \rho]$.

Interaction representation: $\rho(t) = e^{-\imath\mathcal{H}_0 t/\hbar}\tilde{\rho}(t)e^{\imath\mathcal{H}_0 t/\hbar}$.

$$\Rightarrow \frac{\partial\rho}{\partial t} = -\frac{\imath}{\hbar}\Big(\underbrace{\mathcal{H}_0\rho - \rho\mathcal{H}_0}_{[\mathcal{H}_0,\rho]}\Big) + e^{-\imath\mathcal{H}_0 t/\hbar}\frac{\partial\tilde{\rho}}{\partial t}e^{\imath\mathcal{H}_0 t/\hbar}.$$

Substitute these expressions into von Neumann equation:

$$\Rightarrow e^{-\imath\mathcal{H}_0 t/\hbar}\frac{\partial\tilde{\rho}}{\partial t}e^{\imath\mathcal{H}_0 t/\hbar} = -\frac{\imath}{\hbar}\Big(\mathcal{V}(t)e^{-\imath\mathcal{H}_0 t/\hbar}\tilde{\rho}e^{\imath\mathcal{H}_0 t/\hbar} - e^{-\imath\mathcal{H}_0 t/\hbar}\tilde{\rho}e^{-\imath\mathcal{H}_0 t/\hbar}\mathcal{V}(t)\Big).$$

$$\Rightarrow \frac{\partial\tilde{\rho}}{\partial t} = -\frac{\imath}{\hbar}\Big(\underbrace{e^{\imath\mathcal{H}_0 t/\hbar}\mathcal{V}(t)e^{-\imath\mathcal{H}_0 t/\hbar}}_{\tilde{\mathcal{V}}(t)}\tilde{\rho} - \tilde{\rho}\underbrace{e^{\imath\mathcal{H}_0 t/\hbar}\mathcal{V}(t)e^{-\imath\mathcal{H}_0 t/\hbar}}_{\tilde{\mathcal{V}}(t)}\Big) = -\frac{\imath}{\hbar}[\tilde{\mathcal{V}}(t), \tilde{\rho}].$$

From density operator to density matrix:

$$\rho = \sum_{nm}\rho_{nm}|n\rangle\langle m| \quad \Rightarrow \tilde{\rho} = e^{\imath\mathcal{H}_0 t/\hbar}\rho e^{-\imath\mathcal{H}_0 t/\hbar} = \rho_{nm}e^{\imath\mathcal{H}_0 t/\hbar}|n\rangle\langle m|e^{-\imath\mathcal{H}_0 t/\hbar}.$$

$$\Rightarrow \tilde{\rho}_{nm} = \rho_{nm}e^{\imath(\omega_n - \omega_m)t}.$$

Interaction matrix elements: $\tilde{\mathcal{V}}_{nm}(t) = \mathcal{V}_{nm}(t)e^{\imath(\omega_n-\omega_m)t}$.

Von Neumann equation in matrix representation is a set of linear ODEs with time-dependent coefficients:

$$\frac{\partial}{\partial t}\tilde{\rho} = -\frac{\imath}{\hbar}\sum_k\Big(\tilde{\mathcal{V}}_{nk}(t)\tilde{\rho}_{km} - \tilde{\rho}_{nk}\tilde{\mathcal{V}}_{km}(t)\Big).$$

Effect of measurement on pure quantum state:

What is being measured is an observable $\mathcal{A}$ (Hermitian operator).

Eigenbasis of $\mathcal{A}$: $\mathcal{A}|n\rangle = a_n|n\rangle$ with real a_n.

Pure quantum state prior to measuement: $|\psi\rangle = \displaystyle\sum_n |n\rangle\langle n|\psi\rangle$ (normalized).

Action of operator $\mathcal{A}$: $\mathcal{A}|\psi\rangle = \displaystyle\sum_n a_n|n\rangle\langle n|\psi\rangle$.

Expectation value: $\langle\psi|\mathcal{A}|\psi\rangle = \displaystyle\sum_n a_n|\langle n|\psi\rangle|^2 = \sum_n a_n P_n$.

Probability of measuring value $a_n$of observable $\mathcal{A}$: $P_n = |\langle n|\psi\rangle|^2$.

If the state $|\psi\rangle$ is not an eigenstate of the observable $\mathcal{A}$ then the measuement outcome is subject to uncertainty, encoded in a non-vanishing variance:

$$(\Delta\mathcal{A})^2 \doteq \langle\psi|\mathcal{A}^2|\psi\rangle - \langle\psi|\mathcal{A}|\psi\rangle^2 = \sum_n a_n^2 P_n - \left(\sum_n a_n P_n\right)^2 .$$

Projection operators: $\pi_n \doteq |n\rangle\langle n|$.

Post-measurement state: $|\phi\rangle = |n\rangle = \dfrac{\pi_n|\psi\rangle}{\sqrt{P_n}}$.

Note that the basis vectors $|n\rangle$ are only stationary states if the observable $\mathcal{A}$ commutes with the Hamiltonian $\mathcal{H}$.

- $[\mathcal{A},\mathcal{H}] = 0$: $|\phi\rangle$ is stationary if $|\psi\rangle$ is stationary or not.
- $[\mathcal{A},\mathcal{H}] \neq 0$: $|\phi\rangle$ is non-stationary if $|\psi\rangle$ is stationary or not.