Texas Quantum Winter School: Lecture 7 Notes

January 2026

I. Lecture 7

A. Hierarchical Equations of Motion: Derivation of the Influence Functional

The size of closed quantum systems scales exponentially with the addition of degrees of freedom. As this scaling makes such simulations impractical in many situations, a variety of open quantum system methods have arisen with different means of controlling computational cost. There is generally a trade off between computational cost and accuracy, with simpler, Markovian methods such as Lindblad or Redfield dynamics being cheap but not applicable in all cases.

The Hierarchical Equations of Motion (HEOM) is a non-Markovian, numerically exact method of propagating the density matrix of a quantum system in time. Provided that the environment surrounding the system of interest can be described by a set of harmonic oscillators, HEOM is a numerically exact method. We will define the density operator of the system as $\hat{\rho}_t$ and presume the typical separation of the total Hamiltonian into a system and bath component, $\hat{H}_S$ and $\hat{H}_B$ respectively, as well as a coupling Hamiltonian $\hat{H}_I$. We will begin the derivation from the path integral approach to quantum mechanics in which the impact of the bath on $\hat{\rho}_t$ is described by a bath influence functional.

B. Simple HEOM Derivation

In this section, we show the simplest possible derivation of HEOM. We choose the interaction Hamiltonian

$$\hat{H}_{\mathrm{I}} = \hat{s} \otimes \hat{F}, \tag{1}$$

where $\hat{s}$ is some system operator, and $\hat{F}$ is the collective coordinate of the bath. The system Hamiltonian $\hat{H}_{\mathrm{S}}$ can be arbitrarily chosen, and the bath Hamiltonian $\hat{H}_{\mathrm{B}}$ is a set of harmonic oscilators. Within the path-integral formalism, the system density operator at time t is written as

$$\hat{\rho}_t = \underbrace{\int \mathrm{d}\boldsymbol{s}\,\mathrm{d}\boldsymbol{s}'}_{\text{int. system paths}} |s_t\rangle\, \rho_0(s_0, s_0')\; \underbrace{\mathscr{F}_t[\boldsymbol{s}, \boldsymbol{s}']}_{\text{bath influence}}\; \overbrace{\mathcal{G}_t[\boldsymbol{s}, \boldsymbol{s}']}^{\text{free propagation}} \langle s_t'|\,. \tag{2}$$

Note that the 't' subscripts we use simply enumerate each identity that we have resolved in the derivation of Eq.(2), and we have chosen the basis to be the eigenbasis of $\hat{s}$. The influence functional,

$$\mathscr{F}_t[\boldsymbol{s}, \boldsymbol{s}'] = \exp\left\{-\frac{1}{\hbar^2}\int_0^t \mathrm{d}\tau\, s_\tau^{\times} \int_0^\tau \mathrm{d}\sigma \left[s_\sigma^{\times} \underbrace{C_{\mathrm{FF}}^{\mathrm{re.}}(\tau-\sigma)}_{\text{Re[noise corr.]}} + i s_\sigma^{\circ} \underbrace{C_{\mathrm{FF}}^{\mathrm{im.}}(\tau-\sigma)}_{\text{Im[noise corr.]}}\right]\right\}, \tag{3}$$

re-weighs system paths due to the presence of the bath. The free propagator $\mathcal{G}_t$ generates the uncoupled evolution of the system. We define

$$s_t^{\times} \equiv s_t - s_t', \qquad\qquad s_t^{\circ} \equiv s_t + s_t', \tag{4}$$

the difference and sum coordinates of the forward and backward system paths. The simplest derivation of HEOM considers a bath correlation function consisting of a single exponential term;

$$C_{\mathrm{FF}}(t) = \eta e^{-\gamma t}, \tag{5}$$

with $\eta \in \mathbb{C}, \gamma \in \mathbb{R}$. To derive HEOM, we take time derivatives of Eq.(2), and group terms [1]. The influence functional gives

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{F}_t[\boldsymbol{s},\boldsymbol{s}'] = \frac{i}{\hbar}s_t^{\times}\underbrace{\frac{i}{\hbar}\int_0^t s_\tau^{\times}C_{\mathrm{FF}}^{\mathrm{re.}}(t-\tau) + is_\tau^{\circ}C_{\mathrm{FF}}^{\mathrm{im.}}(t-\tau)\mathrm{d}\tau}_{\mathscr{f}_t[\boldsymbol{s},\boldsymbol{s}']}\mathscr{F}_t[\boldsymbol{s},\boldsymbol{s}']. \tag{6}$$

Notice the time–local $\frac{i}{\hbar}s_t^{\times}$ factor in the above expression. This can be brought out of the path integral to give the $\frac{i}{\hbar}\hat{s}^{\times}$ superoperator. The same treatment is unfortunately impossible with the other part of the expression. We instead just define it as $\mathscr{f}_t[\boldsymbol{s},\boldsymbol{s}']$, and continue with differentiation. For the BCF given in Eq.(5)

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{f}_t[\boldsymbol{s},\boldsymbol{s}'] = \frac{i}{\hbar}s_t^{\times}\mathrm{Re}[\eta] - \frac{1}{\hbar}s_t^{\circ}\mathrm{Im}[\eta] - \gamma\mathscr{f}_t[\boldsymbol{s},\boldsymbol{s}']. \tag{7}$$

The first two terms in this expression are time–local and hence the same superoperator treatment can be used to handle them. The other is just a damping constant. These equations show that if we define Auxiliary Density Operators (ADOs)

$$\rho_t^{[n]}(s_t,s_t') := \int \mathrm{d}\boldsymbol{s}\,\mathrm{d}\boldsymbol{s}'\rho_0(s_0,s_0')\left(\mathscr{f}_t[\boldsymbol{s},\boldsymbol{s}']\right)^n\,\mathscr{F}_t[\boldsymbol{s},\boldsymbol{s}']\mathscr{G}_t[\boldsymbol{s},\boldsymbol{s}'], \tag{8}$$

we can obtain a closed set of equations of motion for $\{\rho_t^{[n]}\}$. As we also know the initial condition to be $\rho_0^{[n]} = \rho_0\,\delta_{0n}$, we can now just integrate the EOMs without having to worry about the path integrals. The equations of motion (shown in operator form for clarity) are

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\rho}_t^{[n]} = -\frac{i}{\hbar}\left[\hat{H}_{\mathrm{S}},\hat{\rho}_t^{[n]}\right] - n\gamma\hat{\rho}_t^{[n]} + \frac{i}{\hbar}\left[\hat{s},\hat{\rho}_t^{[n+1]}\right] - \frac{n\mathrm{Im}[\eta]}{\hbar}\left\{\hat{s},\hat{\rho}_t^{[n-1]}\right\} + \frac{in\mathrm{Re}[\eta]}{\hbar}\left[\hat{s},\hat{\rho}_t^{[n-1]}\right], \tag{9}$$

Note that we have obtained a coupled series of differential equations for the auxiliary density operators. HEOM is formally exact provided that there are an infinite number of auxiliary density operators. This is, of course, not practical on a real computer. At a certain cut-off value, N, the series must be truncated, with the point of truncation selected so as to maintain numerical accuracy.

In the case that there are a total of K features in the bath correlation function, the derivation is significantly more complicated and a multi-index, $\overrightarrow{n} = n_1, n_2, n_3 ... n_K$ must be employed to describe the resulting set of ADO's, with each index n_i ascending from 0 to infinity and, necessarily, truncated at N. The system's density matrix is found where all $n_i = 0$. This results in the computational cost of HEOM increasing factorially with the number of exponential terms required to represent the bath correlation function. Recent applications of tensor compression methods to HEOM have succeeded in reducing the scaling.

References

[1] Yoshitaka Tanimura. Numerically "exact" approach to open quantum dynamics: The hierarchical equations of motion (HEOM). *The Journal of Chemical Physics*, 153(2), July 2020.