CHAPTER II

Open System Stochastic Schrödinger Equation

1 Introduction

the open system description via a stochastic Schrödinger equation is based on the assumption that a set of properly generated state vectors $|\psi_\zeta(t)\rangle$ are ready to defined the RDO

$$\hat{\rho}(t) = \frac{1}{N}\sum_\zeta |\psi_\zeta(t)\rangle\langle\psi_\zeta(t)|$$

the $|\psi_\zeta(t)\rangle$ are the solution of a time-dependent Schrödinger equation extended by terms due to the system-reservoir coupling;
those have some random character;
if the related time-dependent but random contributions to the Schrödinger equation are counted by ζ, the RDO is obtained as an average with respect to these random (stochastic) processes;
the determination of the RDO by the various $|\psi_\zeta(t)\rangle$ is called stochastic unraveling of the RDO dynamics;

two variants of stochastic Schrödinger equations exist:
(a) approach based on so-called quantum jumps
(b) approach based quantum state diffusion

while it is of general interest if such a view on open system quantum dynamics is possible there is also a practical (computational) aspect;

let us denote the states used to form density matrix elements as $|a\rangle$;
their total number to be considered is N;
accordingly $N \times N$ density matrix elements have to be computed;
if we expand the stochastic Schrödinger equation with respect to the $|a\rangle$ we need to compute N expansion coefficients;

however, this has to be done several times to carry out the average with respect to the different realizations of the stochastic process;
there are various examples where this number is much smaller than N; it may result much less overall propagation than N^2;

1.1 Unraveling of the RDO Dynamics

non-Markaovian equation of motion for the RDO (mean-field contributions shall not exist; $t_0 = 0$)

$$\frac{\partial}{\partial t}\hat{\rho}(t) = -\frac{i}{\hbar}[H_{\rm S}, \hat{\rho}(t)]_-$$

$$-\sum_{u,v}\int_0^t d\tau\Big(C_{uv}(\tau)\Big[K_u, U_{\rm S}(\tau)K_v\hat{\rho}(t-\tau)U_{\rm S}^+(\tau)\Big]_- - \ C_{vu}(-\tau)\Big[K_u, U_{\rm S}(\tau)\hat{\rho}(t-\tau)K_v U_{\rm S}^+(\tau)\Big]_-\Big)$$

respective RDO dynamics can be obtained by the solutions of the non-Markovian stochastic Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H_{\rm S}|\psi(t)\rangle + \sum_u \eta_u(t)K_u|\psi(t)\rangle - i\hbar\sum_{u,v}\int_0^t d\tau C_{uv}(\tau)K_u U_{\rm S}(\tau)K_v|\psi(t-\tau)\rangle$$

wave function depends on the realization of the complex noise $\eta_u(t)$: $\quad |\psi(t)\rangle \to |\psi(t;\eta)\rangle$
RDO shall follow as the stochastic average

$$\hat{\rho}(t) = <|\psi(t;\eta)\rangle\langle\psi(t;\eta)|>_\eta$$

properties of the complex coloured noise

$$<\eta_u(t)>_\eta = 0 \qquad <\eta_u(t)\eta_u(\tau)>_\eta = 0 \qquad <\eta_u^*(t)\eta_u(\tau)>_\eta = C_{uv}(t-\tau)$$

how this scheme works in detail has to be derived;

2 Quantum Jump Description: Monte Carlo Wave-Function Propagation

the procedure to be described is named quantum jump method in contrast to the quantum diffusion method where the wave function changes continuously in times;
we take the dissipative part of the density operator equation in the Lindblad-form

$$-\mathcal{D}_{\mathrm{L}}\ \hat{\rho}(t) = -\sum_{A} \left\{ \frac{1}{2} \Big(L_A L_A^{+}, \hat{\rho} \Big)_{+} - L_A^{+} \hat{\rho} L_A \right\}$$

it has to be specified separately in which manner the Lindblad-operators L_A^{+} and L_A act and what the meaning of the labels A is;
based on this type of dissipative superoperator one determines a bundle of N different time-dependent wave-functions (state vectors) $|\psi_\eta(t)\rangle$ which are generated according t0 the so-called Monte Carlo Wave-Function (MCWF) method time-step δt by time-step δt; the resulting RDO shall fulfill

$$\frac{\partial}{\partial t}\hat{\rho} = -\frac{i}{\hbar}\Big((H_{\mathrm{S}} + \Delta H)\hat{\rho} - \hat{\rho}(H_{\mathrm{S}} + \Delta H^{+}) \Big) + \sum_{A} L_A^{+} \hat{\rho} L_A$$

the anti-Hermitian contribution

$$\Delta H = -i\hbar \sum_{A} L_A L_A^{+}/2$$

is added to the Hamiltonian H_S;

if one starts with $|\psi(t)\rangle$ at time t one determines the change of the state vector linear in δt; we get a state vector at time $t+\delta t$ which is not normalized to one

$$|\tilde{\psi}(t+\delta t)\rangle = \Big(1 - \frac{i}{\hbar}(H_S + \Delta H)\delta t\Big)|\psi(t)\rangle$$

instead we get the norm as

$$\langle\tilde{\psi}(t+\delta t)|\tilde{\psi}(t+\delta t)\rangle \approx 1 + \langle\psi(t)|\big(\frac{i}{\hbar}(H_S + \Delta H^+) - \frac{i}{\hbar}(H_S + \Delta H^+)|\psi(t)\rangle\delta t = 1 - \delta\mathcal{N}$$

the reduction $\delta\mathcal{N}$ of the proper normalization (linear in δt) reads

$$\delta\mathcal{N} = -\frac{i}{\hbar}\langle\psi(t)|\Delta H^+ - \Delta H|\psi(t)\rangle\delta t = \sum_A \langle\psi(t)|L_A L_A^+|\psi(t)\rangle\delta t \equiv \sum_A \delta\mathcal{N}_A$$

choosing a random number ε between zero and one we introduce a so-called quantum jump if $\varepsilon < \delta\mathcal{N}$ (since $\delta\mathcal{N}$ is a small number the quantum jump is a relatively rare event); this jump has to be carried out according to

$$|\psi(t+\delta t)\rangle = \frac{1}{\sqrt{\delta\mathcal{N}_A/\delta t}} L_A^+|\psi(t)\rangle$$

which operator L_A^+ has to be used is decided in proportion to the probability distribution $\delta\mathcal{N}_A/\delta\mathcal{N}$;

if $\varepsilon > \delta\mathcal{N}$ the obtained state vector is only normalized , and we set at time $t + \delta t$

$$|\psi(t+\delta t)\rangle = \frac{1}{\sqrt{1-\delta\mathcal{N}}}|\tilde{\psi}(t+\delta t)\rangle$$

according to the randomness of this procedure one may generate different time-dependent state vectors $|\psi_\eta(t)\rangle$; then, the density matrix can be constructed as indicated above;

the given procedure has not been directly derived; accordingly we cannot decide if the time-evolution of a single wave function has any meaning; but its reliability to produce the correct RDO is justified by the fact that the RDO generated in this way obeys the standard quantum master equation;

in order to demonstrate this the time-evolution from t to $t + \delta t$ is analyzed;
we consider a $|\psi_\eta(t)\rangle$ of a particular propagation up to time t;
the average at time $t + \delta t$ with respect to the random numbers ε is obtained as (η is not written)

$$< |\psi(t+\delta t)\rangle\langle\psi(t+\delta t)| >= (1-\delta\mathcal{N})\frac{|\tilde{\psi}(t+\delta t)\rangle}{\sqrt{1-\delta\mathcal{N}}}\frac{\langle\tilde{\psi}(t+\delta t)|}{\sqrt{1-\delta\mathcal{N}}} + \delta\mathcal{N}\sum_A \frac{\delta\mathcal{N}_A}{\delta\mathcal{N}}\frac{L_A^+|\psi(t)\rangle}{\sqrt{\delta\mathcal{N}_A/\delta t}}\frac{\langle\psi(t)|L_A}{\sqrt{\delta\mathcal{N}_A/\delta t}}$$

the term $\sim 1 - \delta\mathcal{N}$ corresponds to the averaged contribution of that part of the evolution which proceeds in the absence of quantum jumps (the overall probability is $1 - \delta\mathcal{N}$); quantum jumps are considered via the term $\sim \delta\mathcal{N}$ (the overall probability of quantum jumps is $\delta\mathcal{N}$);

it follows

$$< |\psi(t+\delta t)\rangle\langle\psi(t+\delta t)| >= |\tilde{\psi}(t+\delta t)\rangle\langle\tilde{\psi}(t+\delta t)| + \sum_A L_A^+|\psi(t)\rangle\langle\psi(t)|L_A\delta t$$

$$= \big(1 - i(H_\mathrm{S} + \Delta H)\delta t/\hbar\big)|\psi(t)\rangle\langle\psi(t)|\big(1 + i(H_\mathrm{S} + \Delta H^+)\delta t/\hbar\big) + \sum_A L_A^+|\psi(t)\rangle\langle\psi(t)|L_A\delta t$$

$$\approx |\psi(t)\rangle\langle\psi(t)| - \delta t\frac{i}{\hbar}\big[H_\mathrm{S}, |\psi(t)\rangle\langle\psi(t)|\big]_- - \delta t\frac{1}{2}\sum_A \big[L_A L_A^+, |\psi(t)\rangle\langle\psi(t)|\big]_+ + \delta t\sum_A L_A^+|\psi(t)\rangle\langle\psi(t)|L_A$$

according to the relation

$$\hat{\rho}(t) = \lim_{N\to\infty}\sum_{\eta=1}^N \frac{1}{N}|\psi_\eta(t)\rangle\langle\psi_\eta(t)|$$

we average over all values of $|\psi_\eta(t)\rangle$ and arrive at the original quantum master equation

$$\frac{1}{\delta t}\lim_{N\to\infty}\sum_{\eta=1}^N \frac{1}{N}\Big(|\psi_\eta(t+\delta t)\rangle\langle\psi_\eta(t+\delta t)| - |\psi_\eta(t)\rangle\langle\psi_\eta(t)|\Big) = \frac{\partial}{\partial t}\hat{\rho}(t) = -\frac{i}{\hbar}[H_\mathrm{S}, \hat{\rho}(t)]_- - \mathcal{D}_\mathrm{L}\hat{\rho}(t)$$