MODELLING OPEN QUANTUM SYSTEMS - QUANTUM TRAJECTORY METHODS

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Why study open quantum systems?

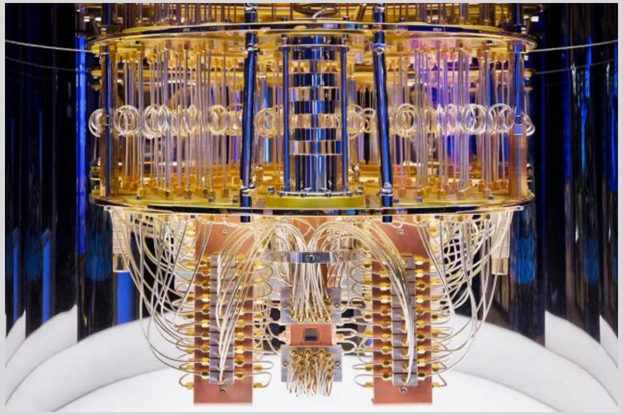

Fig 1: IBM quantum computer

Fig 2: US Capitol building

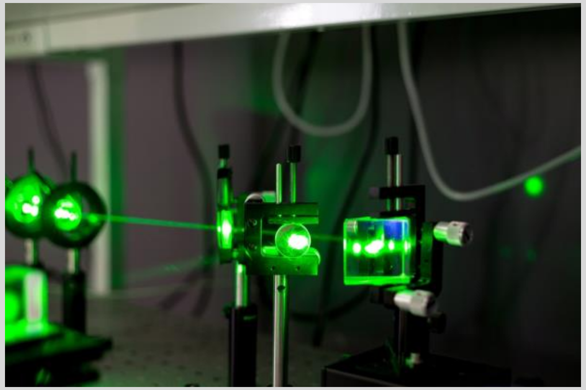

Fig 3: Laser

Closed quantum systems

Schrodinger Equation: $$i\frac{d}{dt}|\varphi(t)\rangle = H(t)|\varphi(t)\rangle$$

$$|\varphi(t)\rangle = U(t,t_0)|\varphi(t_0)\rangle$$

Time-independent Hamiltonian: $$U(t,t_0) = e^{-iH(t-t_0)}$$

Time-dependent Hamiltonian: $$U(t,t_0) = T_{\leftarrow} exp\left[-i\int_{t_0}^{t} ds\, H(s)\right]$$

Mathematical tools for open quantum systems

Density Operator

Pure State: $\rho(t) \equiv |\varphi(t)\rangle\langle\varphi(t)|$

Ensemble: $\rho(t) \equiv \sum_i |\varphi_i(t)\rangle\langle\varphi_i(t)|$

Evolution: $\rho(t) = U(t,t_0)\rho(t_0)U^\dagger(t,t_0)$

Liouville Von-Neumann: $\frac{\partial}{\partial t}\rho(t) = -i[H(t),\rho(t)]$

Expectation: $\langle\hat{O}\rangle = Tr(\hat{O}\rho)$

Interaction Picture

Partitioned Hamiltonian: $H = H_0 + H_I$

Partitioned Unitary Op.: $U(t,t_0) \equiv U_0(t,t_0)U_I(t,t_0)$

Interaction picture operators:

$$\hat{\tilde{O}} \equiv U_0^\dagger(t,t_0)\hat{O}U_0(t,t_0)$$

$$\hat{\tilde{\rho}} \equiv U_I(t,t_0)\rho(t_0)U_I^\dagger(t,t_0) = U_0^\dagger(t,t_0)\rho(t)\,U_0(t,t_0)$$

Open quantum systems

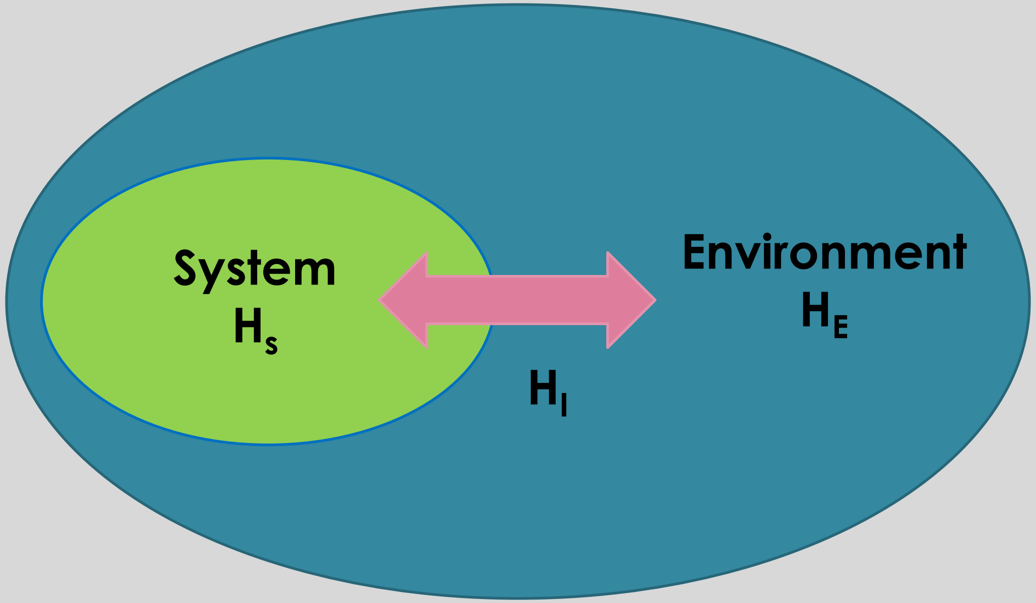

Figure 4: Image showing the general framework of an open quantum system. The open system, S, is the subsystem of a larger combined system, S+E, where E represents the environment. The dynamics of the system and environment degrees of freedom are described by their respective Hamiltonian's, H_s and H_E , with H_I describing the interaction between the two. This image was created using tools in Microsoft Publisher.

Reduced density operator

$$\rho_s(t) = Tr_E(\rho(t))$$

Markovian master equations

$$\frac{\partial}{\partial t}\tilde{\rho}(t) = -i\left[\tilde{H}(t), \tilde{\rho}(t)\right] \quad \Rightarrow \quad \tilde{\rho}(t) = \rho(0) - i\int_0^t ds\left[\tilde{H}_I(t), \tilde{\rho}(t)\right]$$

$$\Longrightarrow \frac{\partial \tilde{\rho}_s}{\partial t} = -iTr_E\left[\tilde{H}_I(t), \tilde{\rho}(0)\right] - \int_0^t ds\, Tr_E\left\{\left[\tilde{H}_I(t), \left[\tilde{H}_I(s), \tilde{\rho}(s)\right]\right]\right\}$$

Assumptions:

1. No correlations
2. Thermal environment
3. The Born Approximation
4. The Markov Approximation

$$\Rightarrow \boxed{\frac{\partial \tilde{\rho}_s(t)}{\partial t} = -\int_0^\infty ds\, Tr_E\left\{\left[\tilde{H}_I(t), \left[\tilde{H}_I(t-s), \tilde{\rho}(s)\otimes\rho_E\right]\right]\right\}}$$

Weak coupling Markovian master equation in the interaction picture

Markovian master equations contd.

$$H_I = \sum_{\alpha} A_\alpha \otimes B_\alpha$$

INTERACTION PICTURE

$$\tilde{H}_I(t) = \sum_{\alpha} A_\alpha(t) \otimes B_\alpha(t)$$

$$A_\alpha(t) = \; e^{iH_S(t)} A_\alpha e^{-iH_S(t)}$$

$$B_\alpha(t) = \; e^{iH_E(t)} B_\alpha e^{-iH_E(t)}$$

Environment correlation functions:

$$C_{\alpha\beta} = \left\langle B_\alpha(t) B_\beta(s) \right\rangle_E = Tr(B_\alpha(t) B_\beta(s) \rho_E)$$

$$[H_E, \rho_E] = 0 \quad \Rightarrow \quad C_{\alpha\beta} = Tr(B_\alpha(t-s) B_\beta \rho_E) \equiv C_{\alpha\beta}(t-s)$$

Markovian master equations contd.

$$\Rightarrow \frac{\partial \tilde{\rho}_S(t)}{\partial t} = -\sum_{\alpha\beta}\int_0^{\infty} d\tau \left(\left[A_\alpha(t), A_\beta(t-\tau)\tilde{\rho}(t)\right]C_{\alpha\beta} + \left[\tilde{\rho}_S(t)A_\beta(t-\tau), A_\alpha(t)\right]C_{\beta\alpha}(-\tau)\right)$$

Recall: $\tilde{\rho}_S(t) = e^{iH_S(t)}\rho_S(t)e^{-iH_S(t)}$

$$\Rightarrow \frac{\partial \rho_S(t)}{\partial t} = -i[H_S, \rho_S(t)] + e^{-iH_S(t)}\left(\frac{\partial \tilde{\rho}_S(t)}{\partial t}\right)e^{iH_S(t)}$$

$$\boxed{\therefore \frac{\partial \rho_S(t)}{\partial t} = -i[H_S, \rho_S(t)] - \sum_{\alpha\beta}\int_0^{\infty} d\tau \left(\left[A_\alpha, A_\beta(-\tau)\rho_S(t)\right]C_{\alpha\beta}(\tau) + \left[\rho_S(t)A_\beta(-\tau), A_\alpha\right]C_{\beta\alpha}(-\tau)\right)}$$

Schrodinger picture master equation

Illustrative example: spin-boson model without tunnelling

System Hamiltonian: $H_S = \frac{\varepsilon}{2}\sigma_z = \frac{\varepsilon}{2}(|e\rangle\langle e| - |g\rangle\langle g|)$

Environment Hamiltonian: $H_E = \sum_{\boldsymbol{k}} \omega_{\boldsymbol{k}} b_{\boldsymbol{k}}^{\dagger} b_{\boldsymbol{k}}$

Interaction Hamiltonian: $H_I = \sum_{\boldsymbol{k}} (g_{\boldsymbol{k}}\sigma_+ b_{\boldsymbol{k}} + g_{\boldsymbol{k}}^{*}\sigma_- b_{\boldsymbol{k}}^{\dagger})$

$$\Rightarrow \boxed{\frac{\partial \rho_S}{\partial t} = -i\frac{\mathcal{E}'}{2}[\sigma_z, \rho_S] + \Gamma(\varepsilon)(N(\varepsilon)+1)(2\sigma_-\rho_S\sigma_+ - \{\sigma_+\sigma_-, \rho_S\}) + \Gamma(\varepsilon)N(\varepsilon)(2\sigma_+\rho_S\sigma_- - \{\sigma_-\sigma_+, \rho_S\})}$$

Optical master equation

Illustrative example: spin-boson model without tunnelling

Bose-Einstein occupation number: $N(\epsilon) = \left(exp\left(\frac{\varepsilon}{k_B T}\right) - 1 \right)^{-1}$

Rates: $\Gamma(\varepsilon) = \pi J(\varepsilon)$

Spectral density: $J(\varepsilon) = \sum_{\boldsymbol{k}} |g_{\boldsymbol{k}}|^2 \delta(\varepsilon - \varepsilon_{\boldsymbol{k}})$

Einstein rate equations

$$\Rightarrow \boxed{\begin{aligned} \dot{\rho}_{ee}(t) &= -2\Gamma(N+1)\rho_{ee}(t) + 2\Gamma N \rho_{gg}(t) \\ \dot{\rho}_{gg}(t) &= -2\Gamma N \rho_{ee}(t) + 2\Gamma N \rho_{gg}(t) \end{aligned}}$$

Illustrative example: Spin-boson model without tunnelling

Driving term: $H_S = \frac{\varepsilon}{2}\sigma_z + \Omega\cos(\omega_l t)\sigma_x$

Optical master equation for a driven system in the rotating frame $\Rightarrow$

$$\boxed{\begin{aligned}\frac{\partial \rho_S'}{\partial t} = -i\frac{v'}{2}[\sigma_z, \rho_S'] - i\frac{\Omega}{2}[\sigma_x, \rho_S'] \\ +\Gamma(\varepsilon)(N(\varepsilon)+1)(2\sigma_-\rho_S\sigma_+ - \{\sigma_+\sigma_-, \rho_S'\}) \\ +\Gamma(\varepsilon)(N(\varepsilon)+1)(2\sigma_-\rho_S\sigma_+ - \{\sigma_+\sigma_-, \rho_S'\})\end{aligned}}$$

Steady state solution:

$$\boxed{\rho_{ee} = \frac{\frac{1}{4}|\Omega|^2}{\Delta^2 + \frac{1}{4}\Gamma^2 + \frac{1}{4}|\Omega|^2}}$$

Variable detuning

Detuning: $\upsilon = \epsilon - \omega_l$

Generalised Rabi frequency: $\widetilde{\Omega} = \sqrt{\upsilon^2 + \Omega^2}$

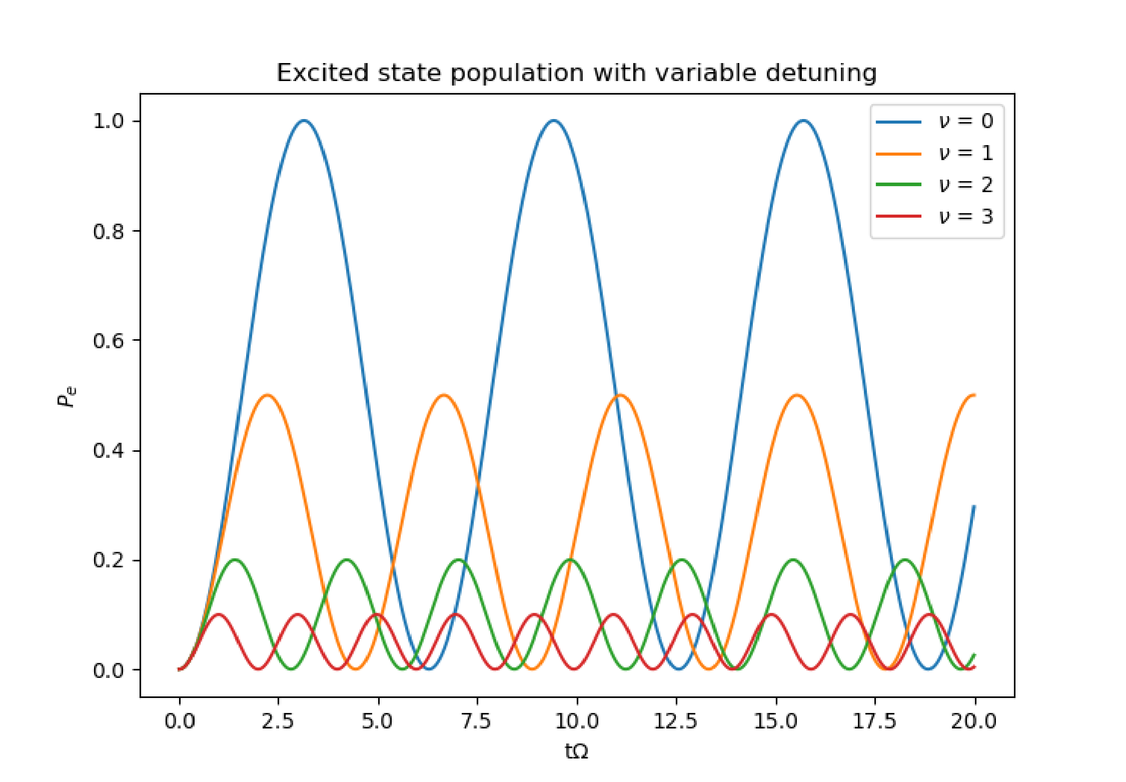

Figure 5: Plots of the excited population with variable detuning

Illustrative example: spin-boson model with tunnelling

Total Hamiltonian

$$\boxed{H_{tot} = \frac{v}{2}\sigma_z + \frac{\Delta}{2}\sigma_x + \sum_{\boldsymbol{k}} \omega_{\boldsymbol{k}} b_{\boldsymbol{k}}^{+} b_{\boldsymbol{k}} + \sum_{\boldsymbol{k}} g_{\boldsymbol{k}}(b_{\boldsymbol{k}}^{+} + b_{\boldsymbol{k}})}$$

Eigenstates of the system Hamiltonian

$$|+\rangle = \sin\left(\frac{\theta}{2}\right)|g\rangle + \cos\left(\frac{\theta}{2}\right)|e\rangle$$

$$|-\rangle = \cos\left(\frac{\theta}{2}\right)|g\rangle - \sin\left(\frac{\theta}{2}\right)|e\rangle$$

$$\theta = tan^{-1}\left(\frac{\Delta}{\varepsilon}\right)$$

Illustrative example: spin-boson model with tunnelling contd.

Master Equation in Lindblad form

$$\frac{\partial \rho_S(t)}{\partial t} = -i[H_S + H_{LS}, \rho_S(t)] + \Gamma_0 \left(P_0 \rho_S(t) P_0 - \frac{1}{2}\{P_0^2, \rho_S(t)\} \right)$$
$$+\Gamma(\eta)\big(1 + N(\eta)\big)\left[P_\eta \rho_S(t) P_\eta^\dagger - \tfrac{1}{2}\left\{P_\eta^\dagger P_\eta, \rho_S(t)\right\}\right]$$
$$+ \Gamma(\eta)\, N(\eta)\left[P_\eta^\dagger \rho_S(t) P_\eta - \tfrac{1}{2}\left\{P_\eta P_\eta^\dagger, \rho_S(t)\right\}\right]$$

$$\eta = \sqrt{v^2 + \Delta^2}$$

P operators: $P_0 = \frac{\epsilon}{\eta}(|+\rangle\langle+| - |-\rangle\langle-|)$ $\quad P_\eta = \frac{\Delta}{\eta}|-\rangle\langle+|$

Rates: $\Gamma_0 = 2\pi \lim_{\epsilon\to 0} J(\varepsilon)\big(1 + N(\epsilon)\big)$ $\quad \Gamma_\eta = 2\pi J(\eta)$

Quantum trajectories technique

$$\boxed{\frac{\partial \rho_S(t)}{\partial t} = -i[H(t), \rho_S(t)] - \frac{1}{2}\sum_m \Gamma_m\left(c_m^\dagger c_m \rho_S(t) + \rho_S(t) c_m^\dagger c_m - 2 c_m \rho_S(t) c_m^\dagger\right)}$$

Markovian master equation in Lindblad form

$$\Rightarrow \frac{\partial \rho_S(t)}{\partial t} = -i\left(H_{\text{eff}}\rho_S(t) - \rho_S(t) H_{\text{eff}}\right) + \sum_m \Gamma_m c_m \rho_S(t) c_m^\dagger$$

Effective Hamiltonian:

$$\boxed{H_{\text{eff}} = H_S - \frac{i}{2}\sum_m \Gamma_m c_m^\dagger c_m}$$

First-order Monte Carlo wavefunction method

1. $$|\psi(t=0)\rangle$$

2. $$\left|\psi^{(1)}(t+\delta t)\right\rangle = e^{-iH_{\mathrm{eff}}\delta t}|\psi(t)\rangle \approx (1 - iH_{\mathrm{eff}}\delta t)|\psi(t)\rangle$$

3. $$\begin{aligned}\left\langle\psi^{(1)}(t+\delta t)\middle|\psi^{(1)}(t+\delta t)\right\rangle &= \left\langle\psi(t)\middle|(1+iH_{\mathrm{eff}}^{\dagger}\delta t)(1-iH_{\mathrm{eff}}\delta t)\middle|\psi(t)\right\rangle \\ &\approx 1 - \delta t\left\langle\psi(t)\middle|i(H_{\mathrm{eff}} - H_{\mathrm{eff}}^{\dagger})\middle|\psi(t)\right\rangle \\ &\equiv 1 - \delta p\end{aligned}$$

$$\begin{aligned}\delta p &= \delta t\sum_{m}\left\langle\psi(t)\middle|c_m^{\dagger}c_m\middle|\psi(t)\right\rangle \\ &\equiv \sum_{m}\delta p_m\end{aligned}$$

First-order Monte Carlo wavefunction method contd.

4. $r_1 \in [0,1]$

a. $r_1 > \delta p \quad \Rightarrow \quad$ 'no jump'

Probability $1 - \delta p$

$$|\psi(t+\delta t)\rangle = \frac{\left|\psi^{(1)}(t+\delta t)\right\rangle}{\sqrt{1-\delta p}}$$

b. $r_1 < \delta p \quad \Rightarrow \quad$ 'jump'

Probability δp

i. $m \in \delta p_m[0,1]$

ii. $r_2 \in [0,1]$

iii. $\Pi_m = \dfrac{\delta p_m}{\delta p}$

iv. $|\psi(t+\delta t)\rangle = \dfrac{c_m|\psi(t)\rangle}{\sqrt{\dfrac{\delta p_m}{\delta t}}}$

Quantum trajectory equivalence to master equation

$$\sigma(t) = \left|\phi(t)\right\rangle\left\langle\phi(t)\right|$$

$$\Rightarrow\ \overline{\sigma(t+\delta t)} = (1-\delta p)\frac{\left|\phi^{(1)}(t+\delta t)\right\rangle}{\sqrt{1-\delta p}}\frac{\left\langle\phi^{(1)}(t+\delta t)\right|}{\sqrt{1-\delta p}} + \delta p\sum_m \Pi_m \frac{c_m\left|\phi(t)\right\rangle}{\sqrt{\frac{\delta p_m}{\delta t}}}\frac{\left\langle\phi(t)\right|c_m^\dagger}{\sqrt{\frac{\delta p_m}{\delta t}}}$$

$$\Rightarrow\ \overline{\sigma(t+\delta t)} = \sigma(t) - i\delta t\left(H_{\text{eff}}\sigma(t) - \sigma(t)H_{\text{eff}}^\dagger\right) + \delta t\sum_m c_m\sigma(t)c_m^\dagger$$

$$\therefore\ \sigma(t) = \lim_{\delta t\to 0}\left(\frac{\overline{\sigma(t+\delta t)} - \sigma(t)}{\delta t}\right) = -i\left(H_{\text{eff}}\sigma(t) - \sigma(t)H_{\text{eff}}^\dagger\right) + \sum_m c_m\sigma(t)c_m^\dagger$$

Quantum trajectories: Spin-boson model without tunnelling

$$\boxed{H_{\text{eff}} = \frac{\upsilon'}{2}\sigma_z + \frac{\Omega}{2}\sigma_x - i\Gamma(\varepsilon)N(\varepsilon)\sigma_-\sigma_+ - i\Gamma(\varepsilon)(1+N(\varepsilon))\sigma_+\sigma_-}$$

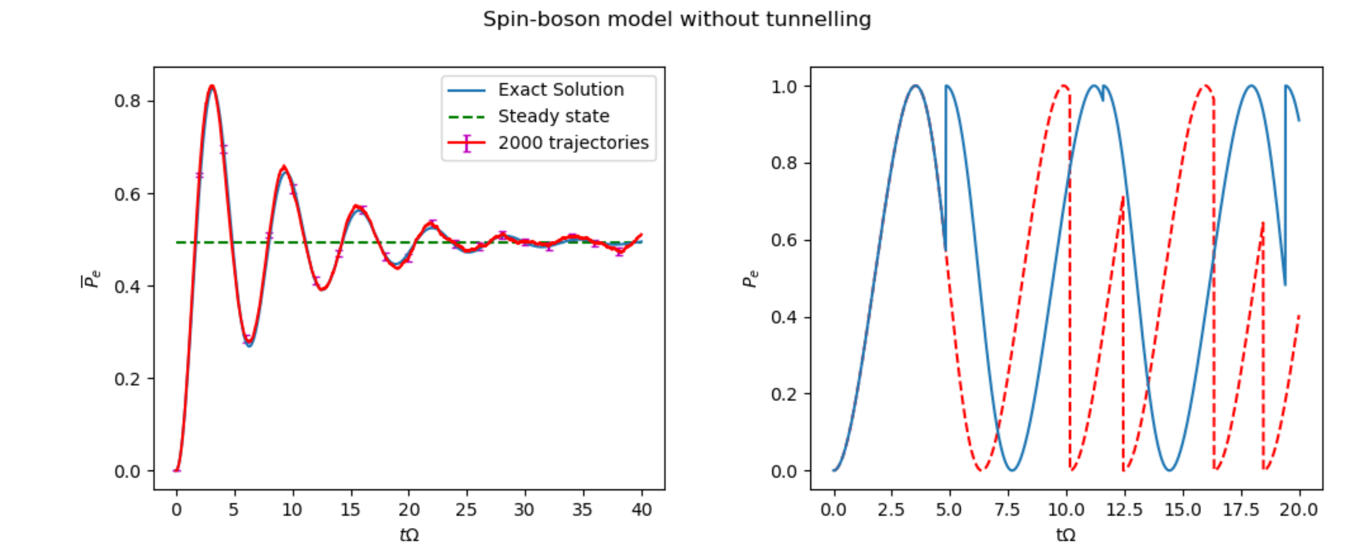

Figure 6: Illustrative example of quantum trajectories for the spin-boson model without tunnelling. Right: probability to find the atom in the excited state, for two random sample trajectories starting in the ground state. Left: population of the excited state averaged over 2000 trajectories (red line), compared with the exact solution found from direct integration of the master equation (blue line) using the Python QuTiP package. The steady state solution is also shown (dashed green line). In both cases we choose detuning υ'= 0, Rabi frequency Ω = 1meV, rate Γ = Ω/6 , optical transition frequency ω = 1eV and temperature T = 298K.

Quantum trajectories: Spin-boson model without tunnelling

$$\boxed{H_{\text{eff}} = H_S - i\frac{\Gamma_0}{2}P_0^2 - i\frac{\Gamma(\eta)}{2}\big(1 + N(\eta)\big)P_\eta^\dagger P_\eta - i\frac{\Gamma(\eta)}{2}N(\eta)P_\eta P_\eta^\dagger}$$

Ohmic spectral density: $J(\varepsilon) = \alpha\varepsilon$

$$\Rightarrow\ \Gamma_0 = 2\pi \lim_{\varepsilon\to 0} \alpha\varepsilon\big(1 + 2N(\varepsilon)\big) \approx 2\pi \lim_{\varepsilon\to 0} \alpha\varepsilon\left(1 + \frac{2k_BT}{\varepsilon}\right) = 4\pi\alpha k_BT$$

$$\left[N(\varepsilon) = \frac{1}{exp\left\{\frac{\varepsilon}{k_BT}\right\} - 1} \approx \frac{k_BT}{\varepsilon}\right]$$

$$\Gamma(\eta) = 2\pi J(\eta) = 2\pi\alpha\eta$$

Quantum trajectories: Spin-boson model without tunnelling contd.

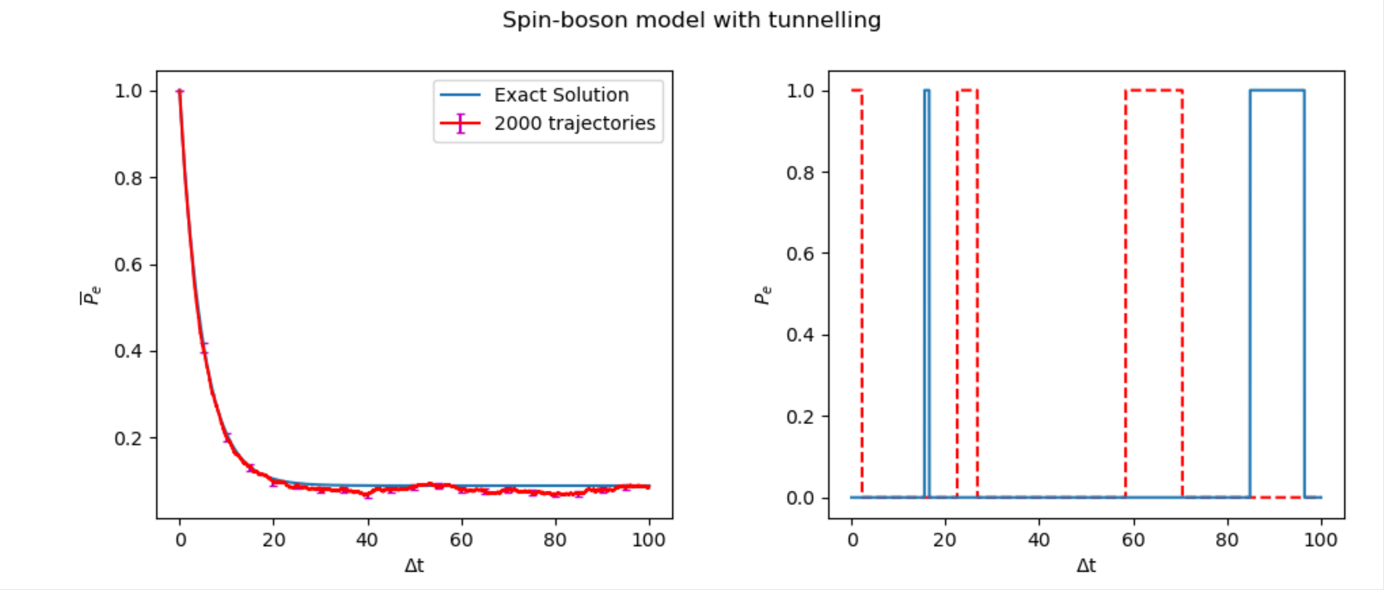

Figure 7: Illustrative example of quantum trajectories for the spin-boson model with tunnelling, working in the energy eigenbasis. Right: population of the excited state for two random sample trajectories propagating in time, one starting in the ground state (solid blue line) and one in the excited state (dashed red line). Left: population of the excited state averaged over 2000 trajectories compared with the exact solution calculated from direct integration of the master equation using the Python QuTiP package [20]. In both cases we choose detuning $\nu = 0$, tunnelling Δ = 1meV, optical transition frequency ω = 1eV, coupling strength $\alpha = \frac{1}{12\pi}$ and temperature T = 5000K.

Errors analysis on trajectory solutions

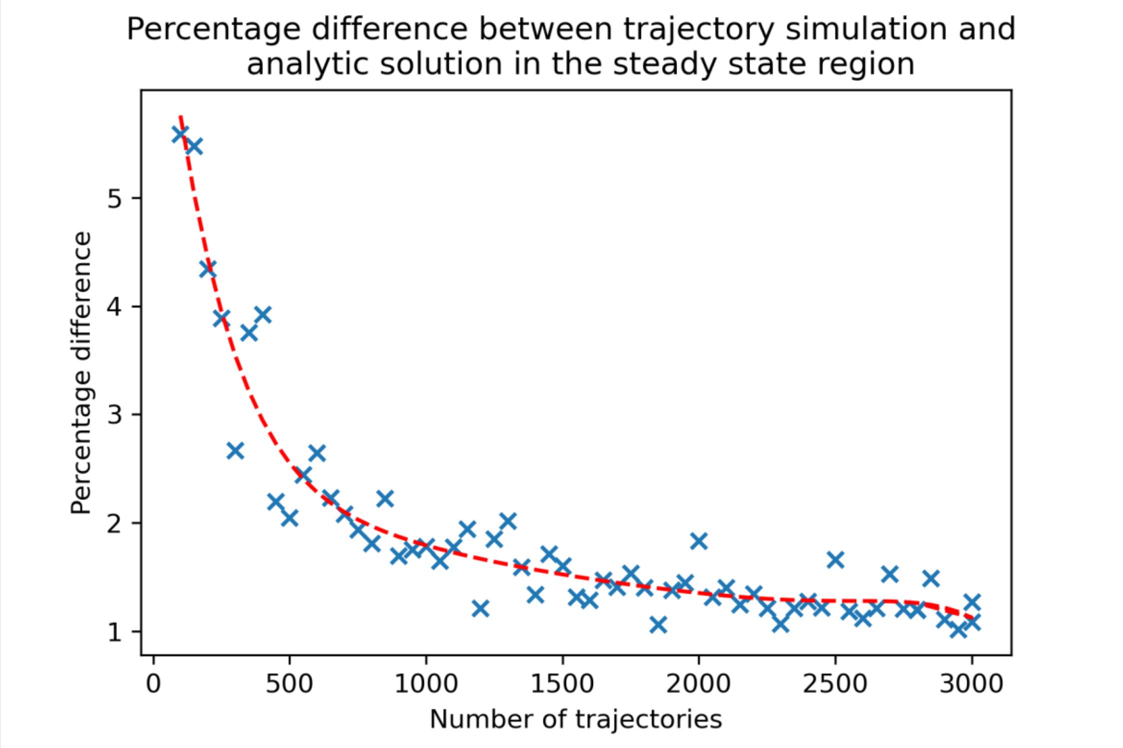

Figure 8: A plot showing how the statistical error (dashed red line) and the absolute error (blue scatter plot), which is the difference between the numerical and analytical result, vary with the number of trajectories.

Statistical error: $$\sigma_A = \frac{\Delta A}{\sqrt{N}}$$

Effect of temperature on thermalisation

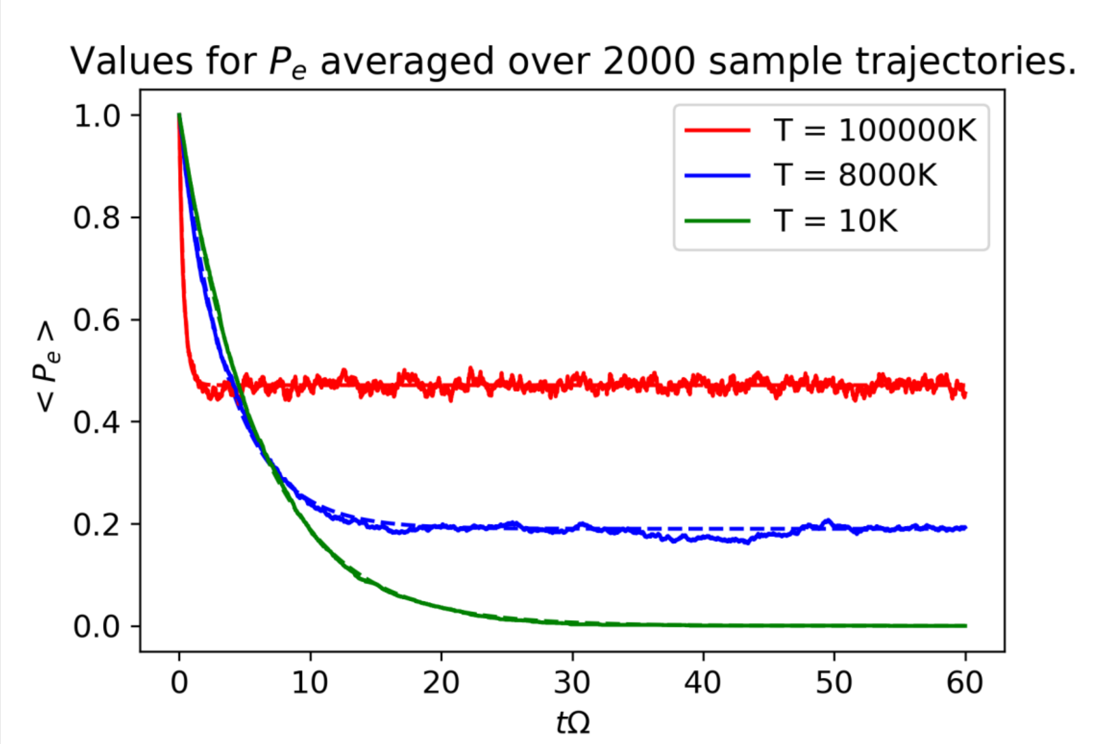

Figure 9: Plot for the average excited state population over 2000 trajectories in the energy eigenbasis of the Optical Bloch system, for temperatures of T =100000K, T = 8000K, T=10K. These are overlaid on the analytical solutions to the Optical master equation for each temperature. In each case we take the tunnelling coefficient Δ = 1meV, optical transition frequency ϵ = 1eV, coupling constant $\alpha = \frac{1}{12\pi}$. The time interval $\Omega\delta$t is taken as 0.01.

Future considerations

- Entropy
- Time dependent Hamiltonians
- Coupling strength