- Crude approximation $U(t+\delta t, t) \approx e^{-iH(t)\delta t}$ can be improved by higher order commutator-free expansion (see, e.g. A. Alvermann, H. Fehske, Journal of Computational Physics 230, 5930 (2011), arXiv: 1102.5071)

↳ Result up to fourth order:

$$\boxed{U(t+\delta t, t) = e^{\frac{1}{2}A_1 + \frac{1}{3}A_2}\, e^{\frac{1}{2}A_1 - \frac{1}{3}A_2} + \mathcal{O}(\delta t^5)}$$

with $A_1 = -i\int_t^{t+\delta t} H(\tilde{\tau})\, d\tilde{\tau}$ and $A_2 = -3i \int_t^{t+\delta t} \left(2\frac{\tilde{\tau}}{\delta t} - 1\right) H(\tilde{\tau})\, d\tilde{\tau}$.

⇝ Integrals are performed numerically with a single Runge-Kutta 4 step to yield:

$$A_1 \underset{+\mathcal{O}(\delta t^5)}{\approx} -i\frac{\delta t}{6}\left(H(t) + H(t+\delta t) + 4H\left(t + \frac{\delta t}{2}\right)\right)$$

$$A_2 \approx -i\frac{\delta t}{2}\left[\left(2\frac{t}{\delta t}-1\right)H(t)+\left(2\frac{t}{\delta t}+1\right)H(t+\delta t)+8\frac{t}{\delta t}H\left(t+\frac{\delta t}{2}\right)\right].$$

↳ Practical recipe:

(i) Compute $K_{n+1}\left(i\left(\frac{A_1}{2}-\frac{A_2}{3}\right), |\Psi(t)\rangle\right)$ with basis Q_- and tridiagonal form T_-.

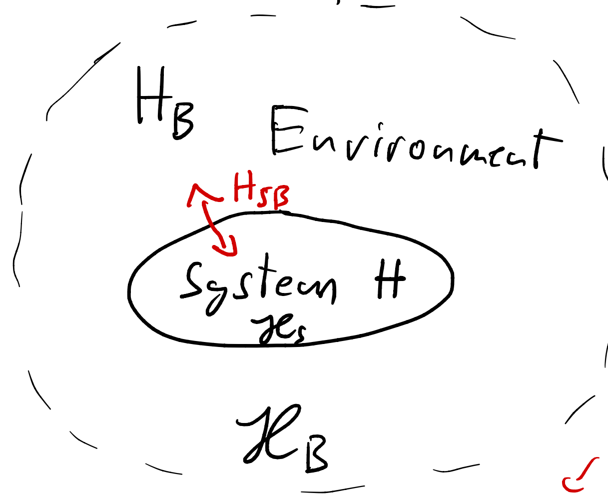
(ii) Update $|\tilde{\Psi}\rangle = Q_- e^{-iT_-}\underbrace{Q_-^{\dagger}|\Psi(t)\rangle}_{\vec{y}_0(t)}$

(iii) Compute $K_{n+1}\left(i\left(\frac{A_1}{2}+\frac{A_2}{3}\right), |\tilde{\Psi}\rangle\right)$ with basis Q_+, and T_+.

(iv) Update $|\Psi(t+\delta t)\rangle = Q_+ e^{-iT_+}\underbrace{Q_+^{\dagger}|\tilde{\Psi}\rangle}_{\tilde{\vec{y}}_0}$

Continue with next time-step.

B.5: Quantum Master Equations and Dissipative Dynamics



- Motivation: System coupled to its environment (bath).

↳ Key ingredients:

- weak coupling (Born)
- bath without memory (Markov)

$$H_{SB} = \sum_\alpha A_\alpha \otimes B_\alpha$$

bath

system

↳ Lindblad master equation:

Liouvillian (superoperator)

for pure states $\rho = |\psi\rangle\langle\psi|$

$\frac{d}{dt}$

$$\dot{\rho} = -i[H, \rho] + \sum_\lambda \left(L_\lambda \rho L_\lambda^\dagger - \frac{1}{2}\{L_\lambda^\dagger L_\lambda, \rho\} \right) = \tilde{\mathcal{L}}(\rho).$$

Operator on $\mathcal{H}_S$

- Vectorize Lindblad master equation as

$$|\dot{\psi}_\rho\rangle = \mathcal{L}\,|\psi_\rho\rangle, \text{ where } |\psi_\rho\rangle = \sum_{i,j} \rho_{ij} \underbrace{|i\rangle}_{\in \mathcal{H}_S} \otimes \underbrace{|j\rangle}_{\in \mathcal{H}_a \cong \mathcal{H}_S}$$

for $\rho = \sum_{i,j} \rho_{i,j} |i\rangle\langle j|$

is the vectorized state on which $\mathcal{L}$ acts as a linear operator.

In coordinate representation, we have:

$$\langle l,m|\dot{\Psi}_\rho\rangle = \dot{\rho}_{lm} = -i\left(H_{ln}\rho_{nm} - \rho_{ln}H_{nm}\right) + \sum_\lambda \Big[L_\lambda^{ln}\rho_{np}L_\lambda^{\dagger pm}$$

$$-\frac{1}{2}\left((L_\lambda^\dagger L_\lambda)_{ln}\,\rho_{nm} + \rho_{ln}\,(L_\lambda^\dagger L_\lambda)_{nm} \right)\Big].$$

In vectorized form, this yields

$$|\dot{\Psi}_\rho\rangle = \mathcal{L}|\Psi_\rho\rangle \text{ with } \mathcal{L} = -i\big(\underset{\mathcal{H}_s}{H} \otimes \underset{\mathcal{H}_a}{\mathbb{1}} - \mathbb{1}\otimes H^T\big) + \sum_\lambda \Big[L_\lambda \otimes L_\lambda^*$$

$$-\frac{1}{2}\left((L_\lambda^\dagger L_\lambda)\otimes \mathbb{1} + \mathbb{1}\otimes (L_\lambda^T L_\lambda^*) \right)\Big].$$

↳ Price to pay:
- Linear operator $\mathcal{L}$ non-Hermitian (Lanczos → Arnoldi)
- $\dim(\mathcal{H}_s) \longrightarrow \dim(\mathcal{H}_s \otimes \mathcal{H}_a) = \left(\dim(\mathcal{H}_s)\right)^2$ (effective doubling in system size)

$\hookrightarrow$ Remedy in part D: Stochastic sampling of dissipative "jumps" (action of L_λ's) allows for algorithm based on pure states in $\mathcal{H}_s$ (quantum trajectories), and thus brings us back to $\dim(\mathcal{H}_s)$.

C.0: The variational principle

- Basic idea: Tame exponential complexity of $|\psi\rangle$ by making a clever variational ansatz

$\approx$?

↳ Key challenges: (i) Identify set of variational states that is <u>unbiased</u> and contains states <u>complex</u> enough that they are close to the true solution

(ii) Devise constructive algorithm that optimizes the variational parameters.