Modeling the metastable dynamics of correlated structures (supplementary materials)

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Master equation

We derive the master equation $\dot{\rho}_S(t) = -i[H_S, \rho_S(t)] - \mathcal{L}\rho_S(t)$ for the reduced density matrix of an open quantum system. First we substitute $H_E = \sum_k \varepsilon_k c_k^\dagger c_k$ and $H_I = \sum_{\alpha k}(\gamma_{\alpha k} c_\alpha^\dagger c_k + \gamma_{\alpha k}^* c_k^\dagger c_\alpha)$ into

$$\frac{d}{dt}\rho_S(t) = -i[H_S, \rho_S(t)] - \int\limits_0^\infty dt' \mathrm{tr}_E[H_I, [e^{-i(H_S+H_E)t'} H_I e^{i(H_S+H_E)t'}, \rho_S(t)\rho_E]] \tag{1}$$

and clarify the action of operator exponents

$$e^{-iH_E t} c_k e^{iH_E t} = e^{i\varepsilon_k t} c_k \qquad e^{-iH_S t} c_\alpha e^{iH_S t} = \sum_{mn} \langle m|c_\alpha|n\rangle e^{-i(E_m - E_n)t} |m\rangle\langle n| \tag{2}$$

Here $|n\rangle$, E_n are eigenstates and eigenergies of H_S obtained by an exact diagonalization. We assume that ρ_E is a Gibbs state and leave only terms with pairs of reservoir operators which do not vanish after taking partial trace. This transforms the non-Liouvillean part into

$$\mathcal{L}\rho_S(t) = \int\limits_0^\infty dt' \mathrm{tr}_E \sum_{\substack{\alpha\beta k \\ mn}} e^{i(E_n - E_m - \varepsilon_k)t'} [\gamma_{\alpha k} c_\alpha^\dagger c_k, [\gamma_{\beta k}^* \langle m|c_\beta|n\rangle c_k^\dagger |m\rangle\langle n|, \rho_S(t)\rho_E]] + \text{h.c.} \tag{3}$$

Taking time integral and partial trace leads to

$$\begin{aligned}\mathcal{L}\rho_S(t) = \pi \sum_{\substack{\alpha\beta k \\ mn}} \delta(E_n - E_m - \varepsilon_k)\gamma_{\alpha k}\gamma_{\beta k}^* \langle m|c_\beta|n\rangle (\bar{f}_k c_\alpha^\dagger |m\rangle\langle n|\rho_S(t) - \\ - f_k c_\alpha^\dagger \rho_S(t)|m\rangle\langle n| - \bar{f}_k |m\rangle\langle n|\rho_S(t) c_\alpha^\dagger + f_k \rho_S(t)|m\rangle\langle n| c_\alpha^\dagger) + \text{h.c.}\end{aligned} \tag{4}$$

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Here $\mathrm{tr}_E(c_k^\dagger c_k \rho_E) = f(\varepsilon_k) = (\exp(\frac{\varepsilon_k - \mu}{T}) + 1)^{-1}$ is a distribution function of particles in the reservoir and $\mathrm{tr}_E(c_k c_k^\dagger \rho_E) = \bar{f}(\varepsilon_k) = (1 + \exp(-\frac{\varepsilon_k - \mu}{T}))^{-1}$. We also introduce hybridization function $J_{\alpha\beta}(\varepsilon) = 2\pi \sum_k \gamma_{\alpha k} \gamma_{\beta k}^* \delta(\varepsilon - \varepsilon_k)$ which allows to rewrite the last expression in the following form

$$\begin{aligned} \mathcal{L}\rho_S(t) = \frac{1}{2} \sum_{\substack{\alpha\beta \\ mn}} J_{\alpha\beta}(\varepsilon_{nm}) \langle m|c_\beta|n\rangle (\bar{f}(\varepsilon_{nm}) c_\alpha^\dagger |m\rangle\langle n| \rho_S(t) - \\ - f(\varepsilon_{nm}) c_\alpha^\dagger \rho_S(t) |m\rangle\langle n| - \bar{f}(\varepsilon_{nm}) |m\rangle\langle n| \rho_S(t) c_\alpha^\dagger + f(\varepsilon_{nm}) \rho_S(t) |m\rangle\langle n| c_\alpha^\dagger) + \text{h.c.} \end{aligned} \tag{5}$$

We note that the matrix structure of $J_{\alpha\beta}(\varepsilon)$ is determined by a hybridization of the reservoir with different localized states. Its dependence on energy is ignored in the wide band approximation. Then we introduce two kinds of transition operators

$$L_\alpha = \sum_{mn} f(\varepsilon_{nm}) \langle m|c_\alpha|n\rangle |m\rangle\langle n| \qquad \bar{L}_\alpha = \sum_{mn} \bar{f}(\varepsilon_{nm}) \langle m|c_\alpha|n\rangle |m\rangle\langle n| \tag{6}$$

They allow to simplify (5) and finally write the master equation as

$$\begin{aligned} \frac{d}{dt}\rho_S(t) = -i[H_S, \rho_S(t)] + \frac{1}{2} \sum_{\alpha\beta} J_{\alpha\beta} (c_\alpha^\dagger \rho_S(t) L_\beta + \bar{L}_\beta \rho_S(t) c_\alpha^\dagger - \\ - c_\alpha^\dagger \bar{L}_\beta \rho_S(t) - \rho_S(t) L_\beta c_\alpha^\dagger) + \text{h.c.} \end{aligned} \tag{7}$$

We note that this derivation is also applicable to bosons if one uses $f(\varepsilon_k) = (\exp(\frac{\varepsilon_k - \mu}{T}) - 1)^{-1}$ and $\bar{f}(\varepsilon_k) = (1 - \exp(-\frac{\varepsilon_k - \mu}{T}))^{-1}$.