Fermionic duality beyond weak coupling: General simplifications of open-system dynamics

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Fermionic duality – functions of microscopic parameters

Problem: The evolutions of states and observables are nontrivially related in open quantum systems due to dissipation and memory effects.

Solution: Fermionic duality

- simple relation for *analytic descriptions* of open system dynamics
- applicable in nonequilibrium, at strong coupling to reservoirs
- **unintuitive but very useful** [1–4]

$$\boxed{\text{Given an analytic result } A(H,V,\mu):\quad \overline{A} \equiv A(-H, iV, -\mu) \text{ can be useful.}}$$

H = system Hamiltonian, V = coupling Hamiltonian, μ = chemical potential(s)

Assumptions:

- Arbitrary local system coupled to noninteracting fermionic reservoirs
- Wide band limit: environment Hamiltonian $H_\mathrm{E} = \int \mathrm{d}\omega\, \omega\, c(\omega)^\dagger c(\omega)$
- Energy-independent, bilinear coupling: $V = \sum_{\alpha l} \int \mathrm{d}\omega\, \tau_{\alpha l}\, \underbrace{c_\alpha(\omega)}_{\text{environment}} \underbrace{d_l^\dagger}_{\text{system}} + h.c.$
- No driving

Propagator – basic duality relation

$$|\rho(t)) = \Pi(t)\,|\rho(0)) = \sum_i \pi_i(t) |\pi_i(t))(\pi_i'(t)|\rho(0)), \qquad |\pi_i(t)) \neq (\pi_i'(t)|^\dagger$$

Duality relation [1]: $\boxed{\Pi^\mathrm{H}(t) \equiv \Pi(t)^\dagger = e^{-\Gamma t} \mathcal{P} \overline{\Pi}(t)\, \mathcal{P}}$ $\qquad \mathcal{P} \equiv (-\mathbb{1})^N \bullet$

- Heisenberg picture evolution: $A(t) = \Pi^\mathrm{H}(t)\, A, \quad (A(t)|\rho(0)) = (A|\rho(t))$
- $H \longrightarrow -H$ inverts local energies, e.g. Coulomb repulsion becomes attractive
- $V \longrightarrow iV$ inverts coupling sign: Coupling rate $\overline{\Gamma} = -\Gamma < 0$
- $e^{-\Gamma t}$: Fix exponential expansion due to inverted coupling
- signs from $\mathcal{P}$: Change sign of the parity-changing part of the evolution

Eigenvector cross-relation: $\quad \pi_j(t) = e^{-\Gamma t}\, \overline{\pi}_i(t)^*, \qquad (\pi_j'(t)| = [\mathcal{P}|\overline{\pi}_i(t))]^\dagger$

$\Rightarrow$ generic eigenmode from trace preservation $\quad \pi_n(t) = e^{-\Gamma t}, \quad |\pi_n(t)) = |(-\mathbb{1})^N)$; $\quad \pi_1(t) = 1, \quad (\pi_1'(t)| = (\mathbb{1}| = \mathrm{tr}\,\bullet$.

$\Rightarrow$ Duality simplifies construction and diagonalization of $\Pi(t)$.

Time-nonlocal quantum master equation

General form: $\dfrac{\mathrm{d}}{\mathrm{d}t}\rho(t) = -i \displaystyle\int_0^t \mathrm{d}s\, \mathcal{K}(t-s)\, \rho(s)$ (Nakajima 1958, Zwanzig 1960)

Similar to $\Pi(t)$:
$$\boxed{\begin{aligned} \mathcal{K}^\mathrm{H}(t) &= \mathcal{K}(t)^\dagger = -e^{-\Gamma t} \mathcal{P} \overline{\mathcal{K}}(t)\, \mathcal{P} + i\Gamma \delta(t - 0^+) \mathcal{I} \\ \hat{\mathcal{K}}^\mathrm{H}(-\omega^*) &= \hat{\mathcal{K}}(\omega)^\dagger = -\mathcal{P} \hat{\overline{\mathcal{K}}}(i\Gamma - \omega^*)\, \mathcal{P} + i\Gamma \mathcal{I} \end{aligned}}$$

$\Rightarrow$ again: eigenvector cross-relation, $\quad \mathcal{K}(t)\, |(-\mathbb{1})^N) = -i\Gamma\delta(t - 0^+) |(-\mathbb{1})^N)$

Time-local quantum master equation

Enforce time-local form: $\dfrac{\mathrm{d}}{\mathrm{d}t}\rho(t) = -i\mathcal{G}(t)\, \rho(t)$ (Tokuyama, Mori, 1975)

Connection Schrödinger $\leftrightarrow$ Heisenberg picture is in general very complicated.

But with duality: $\boxed{\mathcal{G}^\mathrm{H}(t) = \left[\Pi(t)^{-1} \mathcal{G}(t)\, \Pi(t)\right]^\dagger = -\mathcal{P}\overline{\mathcal{G}}(t)\, \mathcal{P} + i\Gamma\mathcal{I}}$

Measurement operators (Kraus)

For every CP-TP evolution of a fermionic quantum system with superselection:

$$\Pi(t) = \sum_e \lambda_e M_e \bullet M_e^\dagger + \sum_o \lambda_o M_o \bullet M_o^\dagger, \qquad \mathrm{tr}\, M_e^\dagger M_e = \mathrm{tr}\, M_o^\dagger M_o = 1, \qquad \lambda_e, \lambda_o > 0$$
$$= \left(\textit{parity preserving } [M_e, (-\mathbb{1})^N] = 0\right) + \left(\textit{parity changing } \{M_o, (-\mathbb{1})^N\} = 0\right)$$

Cross-relation: $\boxed{\begin{aligned} M_e^\dagger &= \overline{M}_{e'}, & \lambda_e &= e^{-\Gamma t}\overline{\lambda}_{e'} \\ M_o^\dagger &= \overline{M}_{o'}, & \lambda_o &= -e^{-\Gamma t}\overline{\lambda}_{o'} \end{aligned}}$ $\longrightarrow$ distinguish parity

$\Rightarrow$ Parity-changing part is *maximally CP-violating* in the dual system.

Sum rules: $\quad \sum_e \lambda_e = \frac{d}{2}\left(1 + e^{-\Gamma t}\right), \qquad \sum_o \lambda_o = \frac{d}{2}\left(1 - e^{-\Gamma t}\right)$

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Jump operators (GKSL / Lindblad)

$$-i\mathcal{G}(t) = -i[H'(t), \bullet] + \sum_{i=e,o} j_i(t) \left[J_i(t) \bullet J_i(t)^\dagger - \tfrac{1}{2}\{J_i(t)^\dagger J_i(t), \bullet\}\right]$$
$$i\mathcal{G}^\mathrm{H}(t) = i[H'^\mathrm{H}(t), \bullet] + \sum_{i=e,o} j_i^\mathrm{H}(t) \left[J_i^\mathrm{H}(t) \bullet J_i^\mathrm{H}(t)^\dagger - \tfrac{1}{2}\{J_i^\mathrm{H}(t) J_i^\mathrm{H}(t)^\dagger, \bullet\}\right]$$

Connection: $\boxed{\begin{aligned} J_e^\mathrm{H}(t) &= \overline{J}_{e'}(t), & j_e^\mathrm{H}(t) &= \overline{j}_{e'}(t) \\ J_o^\mathrm{H}(t) &= \overline{J}_{o'}(t), & j_o^\mathrm{H}(t) &= -\overline{j}_{o'}(t) \end{aligned}}$ $\qquad H'^\mathrm{H} = -\overline{H'}$

$\longrightarrow$ interesting for divisibility, CP, and nonperturbative approximations [5]

Example: Resonant level model

$$H_\mathrm{tot} = \varepsilon d^\dagger d + \int \mathrm{d}\omega\, \omega c_\omega^\dagger c_\omega + \sqrt{\frac{\Gamma}{2\pi}} \int \mathrm{d}\omega\, (d^\dagger c_\omega + c_\omega^\dagger d)$$

Duality for $\Pi(t)$:
$\overline{\Pi}(t) = \Pi(-\varepsilon, -\Gamma, -\mu)$

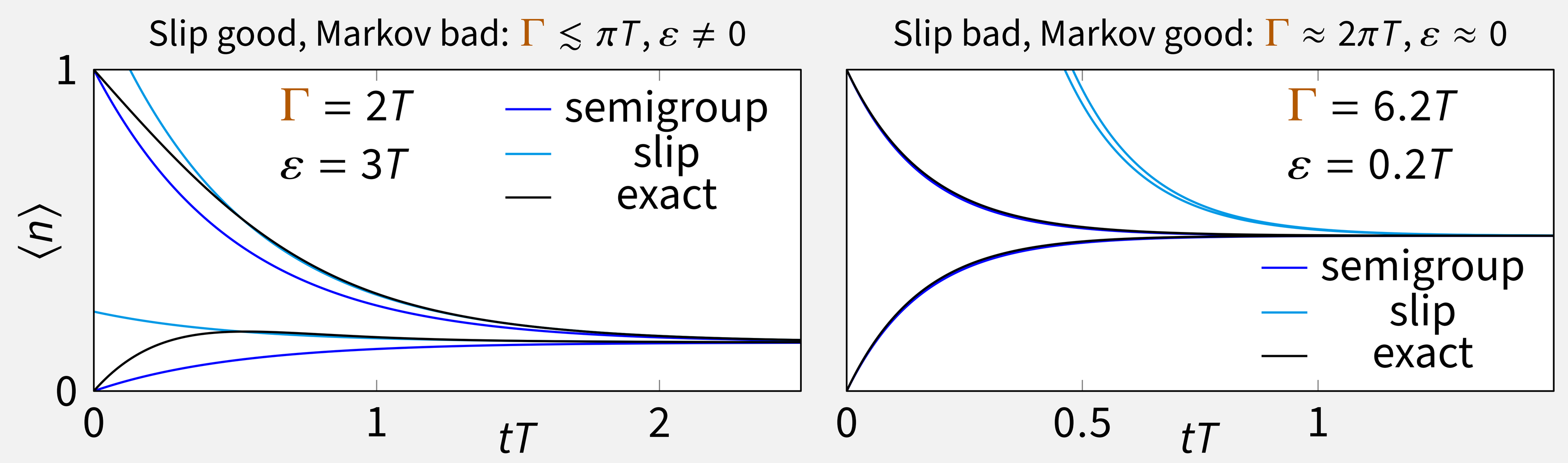
Nontrivial dynamics [6]:
$p(t) = -\overline{p}(t) =$
complicated$(\varepsilon - \mu, \Gamma, T, t)$

$(\pi_i'(t)\|$	$\pi_i(t)$	$\|\pi_i(t))$
$(\mathbb{1}\|$	1	$\frac{1}{2}\left[\|\mathbb{1}) + p(t)\|(-\mathbb{1})^N)\right]$
$(d_\eta^\dagger\|$	$e^{-\frac{1}{2}\Gamma t + i\eta\varepsilon t}$	$\|d_\eta^\dagger)$
$\frac{1}{2}\left[((-\mathbb{1})^N\| + \overline{p}(t)(\mathbb{1}\|\right]$	$e^{-\Gamma t}$	$\|(-\mathbb{1})^N)$

Application: Nonperturbative approximation

Semigroup approximation with initial slip correction [5]: $\quad \Pi^S(t) = e^{-i\mathcal{G}(\infty)\, t}\mathcal{S}$

Construct $\mathcal{S}$ from duality: $\boxed{\begin{gathered} \mathcal{P}\overline{\mathcal{G}(\infty)}^\dagger\mathcal{P} = \mathcal{S}^{-1}\mathcal{G}(\infty)\,\mathcal{S} - i\Gamma\mathcal{I} \\ \mathcal{P}\overline{\mathcal{S}}^\dagger\mathcal{P} = \mathcal{S} \end{gathered}}$



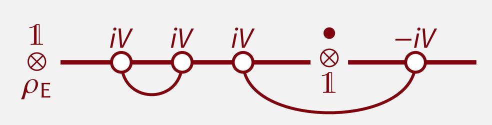
$$\mathcal{S} = -i \sum_g \mathrm{Res}\, \hat{\Pi}(g) \overset{\text{if exists}}{=} \lim_{t\to\infty} e^{i\mathcal{G}(\infty)\, t}\, \Pi(t), \qquad g = \text{ eigenvalues of } \mathcal{G}(\infty)$$

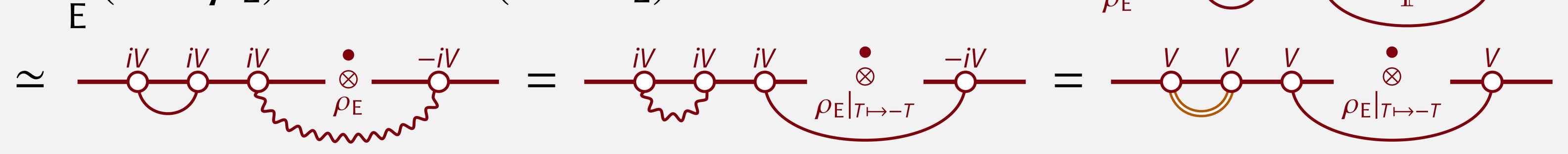
$\longrightarrow$ use fixed point equation [5] $\quad \hat{\mathcal{K}}(g)\, |g) = \mathcal{G}(\infty)\, |g) = g\, |g)$

Slip approximation corrects residues of selected poles: $\quad \mathrm{Res}\, \hat{\Pi}(g) = \mathrm{Res}\, \hat{\Pi}^S(g)$

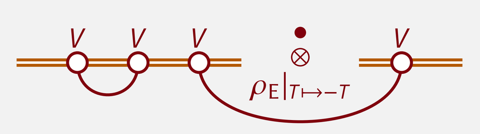
Simpler derivation of fermionic duality

$$\Pi(H, V, \mu, t)^\dagger$$
$$= \mathrm{tr}_\mathrm{E} (\mathbb{1} \otimes \rho_\mathrm{E}) e^{i(H + H_\mathrm{E} + V)t} (\bullet \otimes \mathbb{1}_\mathrm{E}) e^{-i(H + H_\mathrm{E} + V)t} \simeq \tag{1}$$





$$= \mathrm{tr}_\mathrm{E}\, e^{i(H + H_\mathrm{E})t + Vt} (\bullet \otimes \rho_\mathrm{E}|_{T\mapsto -T}) e^{-i(H + H_\mathrm{E})t + Vt} + \text{ redressed versions} \tag{2}$$
$$= e^{-\Gamma t}\, \mathrm{tr}_\mathrm{E}\, e^{i(H + H_\mathrm{E})t + Vt} (\bullet \otimes \rho_\mathrm{E}|_{T\mapsto -T}) e^{-i(H + H_\mathrm{E})t + Vt} \simeq \tag{3}$$



$$= e^{-\Gamma t}\, \mathrm{tr}_\mathrm{E}\, e^{i(H - H_\mathrm{E})t + Vt} (\bullet \otimes \overline{\rho}_\mathrm{E}) e^{-i(H - H_\mathrm{E})t + Vt} \qquad \overline{\rho}_\mathrm{E} \equiv \rho_\mathrm{E}|_{\mu\mapsto -\mu} = \rho_\mathrm{E}\Big|_{\substack{T\mapsto -T \\ H_\mathrm{E}\mapsto -H_\mathrm{E}}} \tag{4}$$
$$= e^{-\Gamma t} (-\mathbb{1})^N\, \mathrm{tr}_\mathrm{E}\, e^{-i(-H + H_\mathrm{E} - iV)t} (-\mathbb{1})^N (\bullet \otimes \overline{\rho}_\mathrm{E}) e^{i(-H + H_\mathrm{E} - iV)t} \tag{5}$$
$$= e^{-\Gamma t} \mathcal{P}\, \Pi(-H, -iV, -\mu, t)\, \mathcal{P} \tag{6}$$

(1)$\longrightarrow$(2) Define: $\overset{1}{\circ}\;\overset{2}{\circ} \equiv -\overset{1}{\circ}\;\overset{2}{\circ} \equiv \delta_{1\bar{2}} - \overset{1}{\circ}\;\overset{2}{\circ} = \overset{1}{\circ}\;\overset{2}{\circ}\Big|_{T\mapsto -T}$
with Wick contractions $\rho_\mathrm{E}\overset{1}{\circ}\;\overset{2}{\circ} = \mathrm{tr}_\mathrm{E}\, \rho_\mathrm{E} c_1 c_2 = \delta_{1\bar{2}} - \mathrm{tr}_\mathrm{E}\, c_1 \rho_\mathrm{E} c_2 = \overset{1}{\circ}\,\rho_\mathrm{E}\,\overset{2}{\circ}$

(2)$\longrightarrow$(3) Extra contractions $\quad \sum_{12} \delta_{1\bar{2}}\, e^{i\omega_1(t_2 - t_1)} = \int \mathrm{d}\omega\, e^{i\omega(t_2 - t_1)} = 2\pi\delta(t_2 - t_1)$:
lead to trivial factor $e^{-\Gamma t/2}$ for forward and backward evolution

(3)$\longrightarrow$(4) Transform reservoir basis: $\quad |\omega\rangle_\alpha \mapsto |-\omega\rangle_\alpha, \quad H_E \mapsto -H_E, \quad \rho_E|_{T\mapsto -T} \mapsto \overline{\rho}_E$

(4)$\longrightarrow$(5) Invert sign of V using fermion parity and $[H, (-\mathbb{1})^N] = 0$

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