ICE-10, VALENCIA, 24/10/25

POTENTIAL RENORMALISATION, LAMB SHIFT & MEAN-FORCE GIBBS STATE–

to shift or not to shift? *

LUIS A. CORREA

* LAC & Glatthard, Quantum 9, 1868 (2025)


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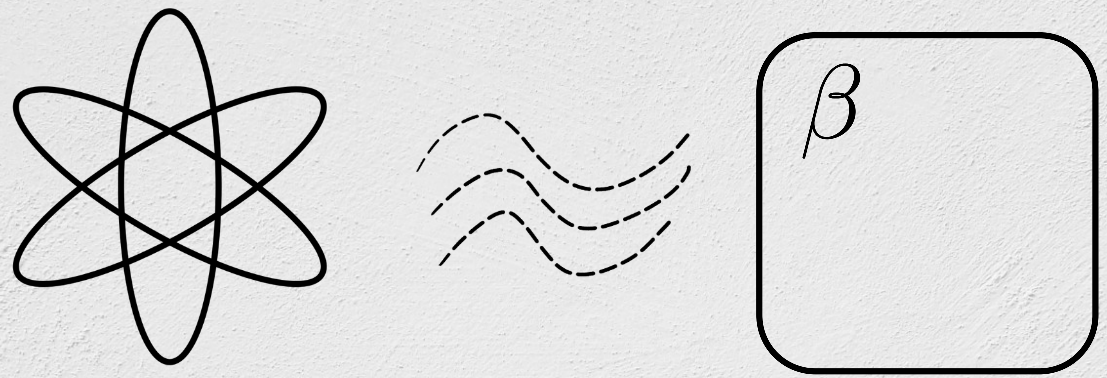
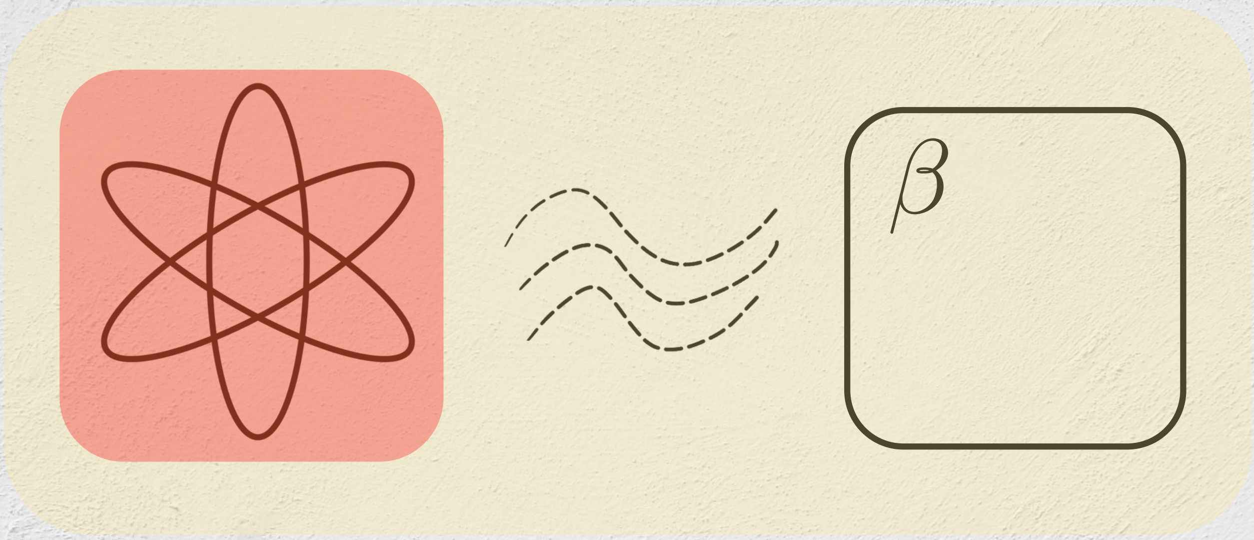


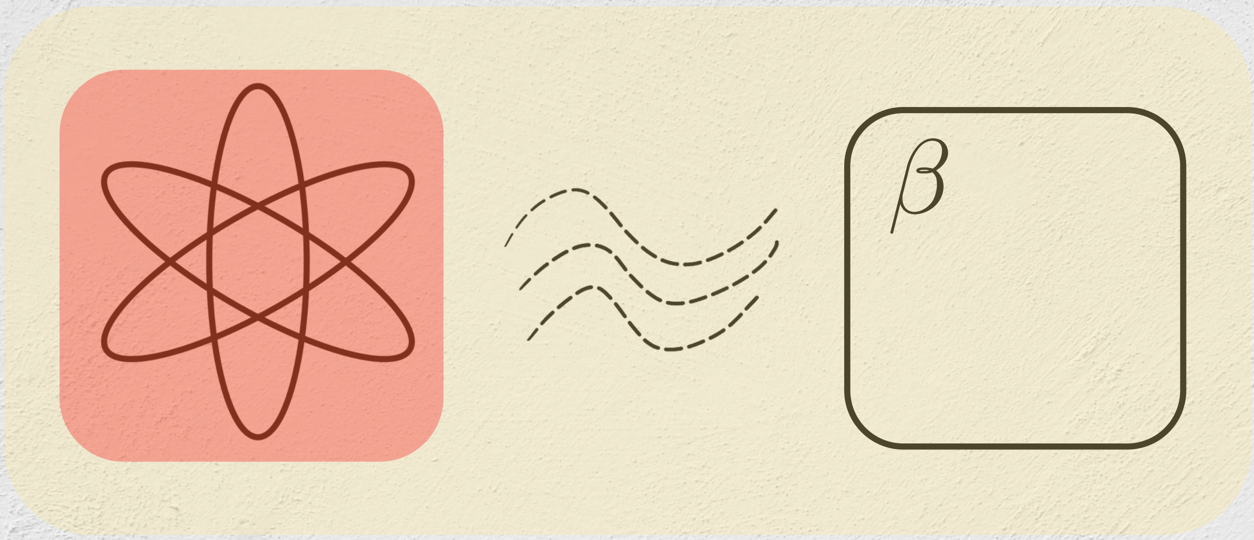
$$\boldsymbol{H}_{\mathrm{tot}} = \boldsymbol{H}_{\mathrm{S}} + \zeta\, \boldsymbol{S} \otimes \boldsymbol{B} + \boldsymbol{H}_{B}$$



$$\boldsymbol{H}_{\text{tot}} = \boldsymbol{H}_{\text{S}} + \zeta\, \boldsymbol{S} \otimes \boldsymbol{B} + \boldsymbol{H}_B$$

mean-force
Gibbs state

$$\boldsymbol{\varrho}_S \xrightarrow[t\to\infty]{} \mathrm{tr}_B\, e^{-\beta \boldsymbol{H}_{\text{tot}}} \propto \boldsymbol{\tau}_{MF}$$



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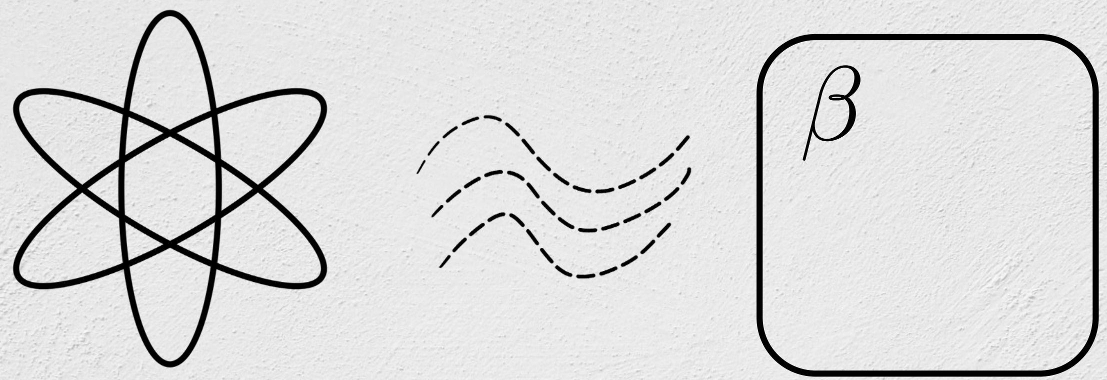
mean-force Gibbs state

$$\boldsymbol{\varrho}_S \xrightarrow[t\to\infty]{} \mathrm{tr}_B\, e^{-\beta \boldsymbol{H}_{\text{tot}}} \propto \boldsymbol{\tau}_{MF}$$

reorganisation energy $\mathcal{O}(\zeta^2)$

$$\boldsymbol{\varrho}_S(t \to \infty) \underset{\beta \ll \omega_0}{\sim} e^{-\beta\,(\boldsymbol{H}_S - Q\,\boldsymbol{S}^2)}$$

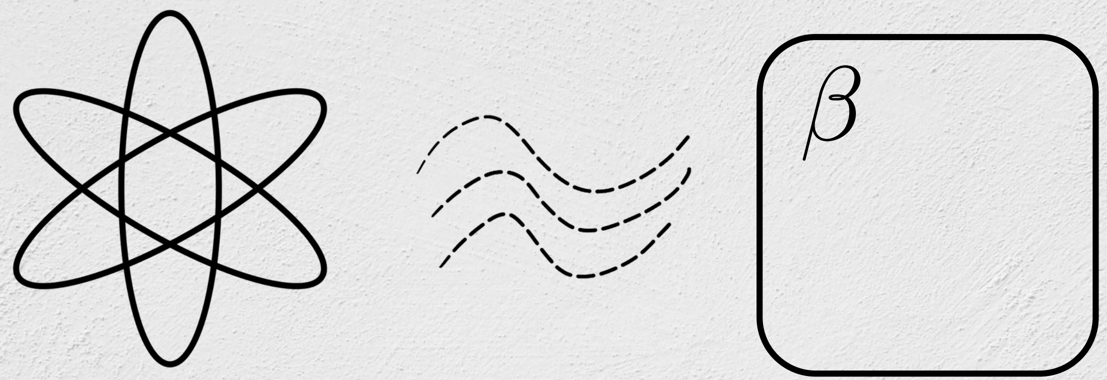
Cerisola et al., NJP 22, 053032 (2025)



renormalised Hamiltonian

$$\boldsymbol{\varrho}_S(t \to \infty) \underset{\beta \ll \omega_0}{\sim} e^{-\beta\,\boxed{(\boldsymbol{H}_S - Q\,\boldsymbol{S}^2)}}$$

Caldeira & Leggett, Ann. Physics 149, 374 (1983)



with counter term	$\boldsymbol{H}_S^{(0)} + Q\,\boldsymbol{S}^2$	$\boldsymbol{H}_S^{(0)}$
no counter term	$\boldsymbol{H}_S^{(0)}$	$\boldsymbol{H}_S^{(0)} - Q\,\boldsymbol{S}^2$
	microscopic Hamiltonian	renormalised Hamiltonian

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$$\frac{d\tilde{\boldsymbol{\varrho}}}{dt} = -i\zeta[\tilde{\boldsymbol{V}}(t), \tilde{\boldsymbol{\varrho}}(t)] := \zeta\, \tilde{\boldsymbol{\mathcal{L}}}(t)\, \tilde{\boldsymbol{\varrho}}(t)$$

$$\tilde{\boldsymbol{\varrho}}(t) = \boldsymbol{\varrho}(0) + \zeta \int_0^t ds\, \tilde{\mathcal{L}}(s)\, \tilde{\boldsymbol{\varrho}}(s)$$

$$\boldsymbol{\varrho}(0) = \boldsymbol{\varrho}_S(0)\boldsymbol{\varrho}_B$$

$$\mathrm{tr}\, \boldsymbol{\varrho}(0)\, \boldsymbol{V} = 0$$

$$\frac{d\tilde{\boldsymbol{\varrho}}_S}{dt} = \zeta^2 \int_0^t ds\, \mathrm{tr}_B\, \tilde{\boldsymbol{\mathcal{L}}}(t)\, \tilde{\boldsymbol{\mathcal{L}}}(t-s)\, \tilde{\boldsymbol{\varrho}}_S(t)\boldsymbol{\varrho}_B + \mathcal{O}(\zeta^3)$$

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Markov approximation

$$\frac{d\tilde{\boldsymbol{\varrho}}_S}{dt} = \zeta^2 \int_0^\infty ds\,\mathrm{tr}_B\,\tilde{\mathcal{L}}(t)\,\tilde{\mathcal{L}}(t-s)\,\tilde{\boldsymbol{\varrho}}_S(t)\boldsymbol{\varrho}_B + \mathcal{O}(\zeta^3)$$

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Redfield equation

$$\frac{d\tilde{\boldsymbol{\varrho}}}{dt} = -i\zeta[\tilde{\boldsymbol{V}}(t), \tilde{\boldsymbol{\varrho}}(t)] := \zeta\, \tilde{\mathcal{L}}(t)\, \tilde{\boldsymbol{\varrho}}(t)$$

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Redfield equation

$$\frac{d\boldsymbol{\varrho}_S}{dt} = -i[\boldsymbol{H}_S + \boldsymbol{\Delta}_{\boldsymbol{H}_S}, \boldsymbol{\varrho}_S] + \mathcal{R}_{\boldsymbol{H}_S}\, \boldsymbol{\varrho}_S$$

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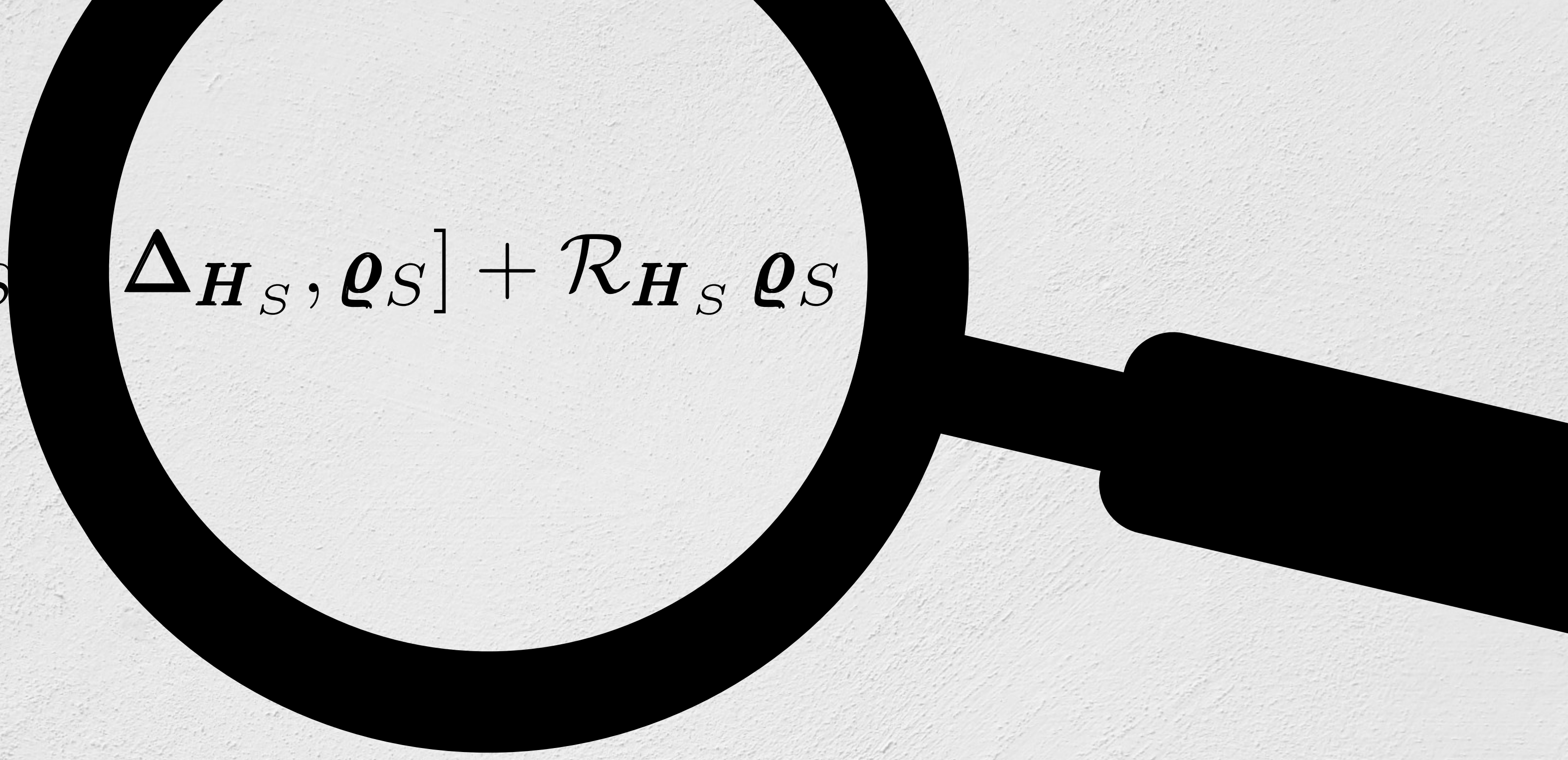

$$\begin{aligned}\Gamma_\omega = \int_0^\infty ds\, e^{i\,\omega\, s}\, \mathrm{tr}\, \tilde{\boldsymbol{B}}(t)\tilde{\boldsymbol{B}}(t-s)\boldsymbol{\varrho}_{\boldsymbol{B}} \\ = \frac{1}{2}\gamma(\omega) + i\, S(\omega)\end{aligned}$$

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$$= \frac{1}{2}\gamma(\omega) + i\, S(\omega)$$

decay rate

Lamb shift

$\mathcal{O}(\zeta^2)$

$$\frac{d\boldsymbol{\varrho}_S}{dt} = -i[\boldsymbol{H}_S + \boldsymbol{\Delta}_{\boldsymbol{H}_S}, \boldsymbol{\varrho}_S] + \mathcal{R}_{\boldsymbol{H}_S}\,\boldsymbol{\varrho}_S$$

$$= -i[\boldsymbol{H}_S + \boldsymbol{\Delta}^{(\gamma)}_{\boldsymbol{H}_S} + \boldsymbol{\Delta}^{(S)}_{\boldsymbol{H}_S}, \boldsymbol{\varrho}_S] + \mathcal{R}^{(\gamma)}_{\boldsymbol{H}_S}\,\boldsymbol{\varrho}_S + \mathcal{R}^{(S)}_{\boldsymbol{H}_S}\,\boldsymbol{\varrho}_S$$

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$$= \underbrace{\frac{1}{2}\gamma(\omega)}_{\text{decay rate}} + \underbrace{i\,S(\omega)}_{\text{Lamb shift}}$$

$\mathcal{O}(\zeta^2)$

$$\frac{d\boldsymbol{\varrho}_S}{dt} = -i[\boldsymbol{H}_S + \boldsymbol{\Delta}^{(\gamma)}_{\boldsymbol{H}_S} + \boldsymbol{\Delta}^{(S)}_{\boldsymbol{H}_S}, \boldsymbol{\varrho}_S] + \mathcal{R}^{(\gamma)}_{\boldsymbol{H}_S}\,\boldsymbol{\varrho}_S + \mathcal{R}^{(S)}_{\boldsymbol{H}_S}\,\boldsymbol{\varrho}_S$$

How does one derive master equations?

$$\frac{d\boldsymbol{\varrho}_S}{dt} = -i[\boldsymbol{H}_R + \boldsymbol{\Delta}^{(\gamma)}_{\boldsymbol{H}_R} + \boldsymbol{\Delta}^{(S)}_{\boldsymbol{H}_R}, \boldsymbol{\varrho}_S] + \mathcal{R}^{(\gamma)}_{\boldsymbol{H}_R}\boldsymbol{\varrho}_S + \mathcal{R}^{(S)}_{\boldsymbol{H}_R}\boldsymbol{\varrho}_S$$

How does one derive master equations?

* Substract the reorganisation energy from the microscopic Hamiltonian and derive the master equation in that basis.

	$\boldsymbol{H}_S$	$\boldsymbol{H}_R$
with counter term	$\boldsymbol{H}^{(0)}_S + Q\,\boldsymbol{S}^2$	$\boldsymbol{H}^{(0)}_S$
no counter term	$\boldsymbol{H}^{(0)}_S$	$\boldsymbol{H}^{(0)}_S - Q\,\boldsymbol{S}^2$

$$\frac{d\boldsymbol{\varrho}_S}{dt} = -i[\boldsymbol{H}_R + \boldsymbol{\Delta}^{(\gamma)}_{\boldsymbol{H}_R} + \cancel{\boldsymbol{\Delta}^{(S)}_{\boldsymbol{H}_R}}, \boldsymbol{\varrho}_S] + \mathcal{R}^{(\gamma)}_{\boldsymbol{H}_R}\boldsymbol{\varrho}_S + \cancel{\mathcal{R}^{(S)}_{\boldsymbol{H}_R}\boldsymbol{\varrho}_S}$$

How does one derive master equations?

* Substract the reorganisation energy from the microscopic Hamiltonian and derive the master equation in that basis.

* Vanish all the Lamb shift terms.

$$\frac{d\boldsymbol{\varrho}_S}{dt} = -i[\boldsymbol{H}_R + \boldsymbol{\Delta}^{(\gamma)}_{\boldsymbol{H}_R}, \boldsymbol{\varrho}_S] + \mathcal{R}^{(\gamma)}_{\boldsymbol{H}_R}\boldsymbol{\varrho}_S$$

How does one derive master equations?

* Substract the reorganisation energy from the microscopic Hamiltonian and derive the master equation in that basis.

* Vanish all the Lamb shift terms.

AND IT WORKS!

... but why?

... and when?

OUTLINE

1. ~~Potential renormalisation and mean-force Gibbs state.~~
2. ~~The Lamb shift.~~
3. To shift or not to shift?
4. The harmonic oscillator.

$$\boldsymbol{H}_S = (\boldsymbol{H}_S - \delta\boldsymbol{H}) + \delta\boldsymbol{H} := \boldsymbol{H}_R + \delta\boldsymbol{H}$$

$\mathcal{O}(\zeta^2)$

$$\frac{d\boldsymbol{\varrho}_S}{dt} = -i[\boldsymbol{H}_S + \boldsymbol{\Delta}^{(\gamma)}_{\boldsymbol{H}_S} + \boldsymbol{\Delta}^{(S)}_{\boldsymbol{H}_S}, \boldsymbol{\varrho}_S] + \mathcal{R}^{(\gamma)}_{\boldsymbol{H}_S}\,\boldsymbol{\varrho}_S + \mathcal{R}^{(S)}_{\boldsymbol{H}_S}\,\boldsymbol{\varrho}_S$$

LAC & Glatthard, Quantum 9, 1868 (2025)
Glatthard et al., PRE 112, 024109 (2025)

$$\boldsymbol{H}_S = (\boldsymbol{H}_S - \delta\boldsymbol{H}) + \delta\boldsymbol{H} := \boldsymbol{H}_R + \overbrace{\delta\boldsymbol{H}}^{\mathcal{O}(\zeta^2)}$$

$$\frac{d\boldsymbol{\varrho}_S}{dt} = -i[\boldsymbol{H}_S + \boldsymbol{\Delta}^{(\gamma)}_{\boldsymbol{H}_R} + \boldsymbol{\Delta}^{(S)}_{\boldsymbol{H}_R}, \boldsymbol{\varrho}_S] + \mathcal{R}^{(\gamma)}_{\boldsymbol{H}_R}\boldsymbol{\varrho}_S + \mathcal{R}^{(S)}_{\boldsymbol{H}_R}\boldsymbol{\varrho}_S + \mathcal{O}(\zeta^3)$$

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$$\boldsymbol{H}_S = (\boldsymbol{H}_S - Q\,\boldsymbol{S}^2) + Q\,\boldsymbol{S}^2 := \boldsymbol{H}_R + \underbrace{Q\,\boldsymbol{S}^2}_{\mathcal{O}(\zeta^2)}$$

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$$\boldsymbol{H}_S = (\boldsymbol{H}_S - Q\,\boldsymbol{S}^2) + Q\,\boldsymbol{S}^2 := \boldsymbol{H}_R + Q\,\underset{\mathcal{O}(\zeta^2)}{\boldsymbol{S}^2}$$

Step 1

$$\frac{d\boldsymbol{\varrho}_S}{dt} = -i[\boldsymbol{H}_S + \boldsymbol{\Delta}^{(\gamma)}_{\boldsymbol{H}_R} + \boldsymbol{\Delta}^{(S)}_{\boldsymbol{H}_R}, \boldsymbol{\varrho}_S] + \mathcal{R}^{(\gamma)}_{\boldsymbol{H}_R}\,\boldsymbol{\varrho}_S + \mathcal{R}^{(S)}_{\boldsymbol{H}_R}\,\boldsymbol{\varrho}_S + \mathcal{O}(\zeta^3)$$

Hartmann & Strunz, Quantum 4, 347 (2020)

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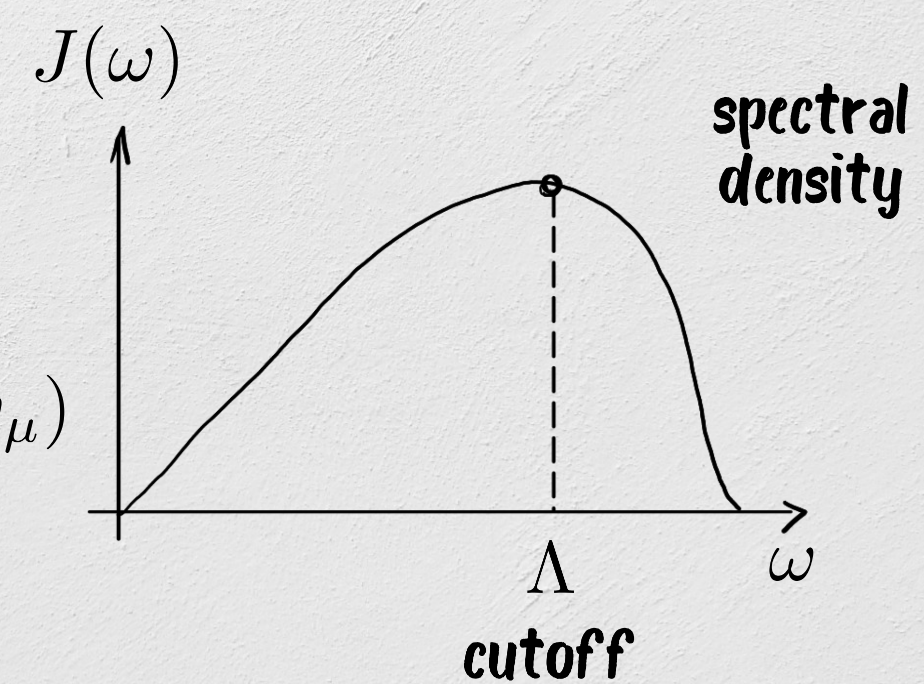
$$\boldsymbol{B} = \sum_\mu g_\mu \boldsymbol{x}_\mu$$

$$J(\omega) = \sum_\mu \frac{g_\mu^2}{2\,m_\mu\,\omega_\mu}\,\delta(\omega - \omega_\mu)$$



Hartmann & Strunz, Quantum 4, 347 (2020)

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$\mathcal{O}(\zeta^2)$

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Step 2

$\omega/\Lambda \ll 1$

(adiabatic limit)

$$-i[\boldsymbol{\Delta}^{(S)}_{\boldsymbol{H}_R}, \boldsymbol{\varrho}_S] + \mathcal{R}^{(S)}_{\boldsymbol{H}_R}\boldsymbol{\varrho}_S \sim -i[-Q\,\boldsymbol{S}^2, \boldsymbol{\varrho}_S]$$

$$\boldsymbol{H}_S = (\boldsymbol{H}_S - Q\,\boldsymbol{S}^2) + Q\,\boldsymbol{S}^2 := \boldsymbol{H}_R + \overset{\mathcal{O}(\zeta^2)}{Q\,\boldsymbol{S}^2}$$

Step 1

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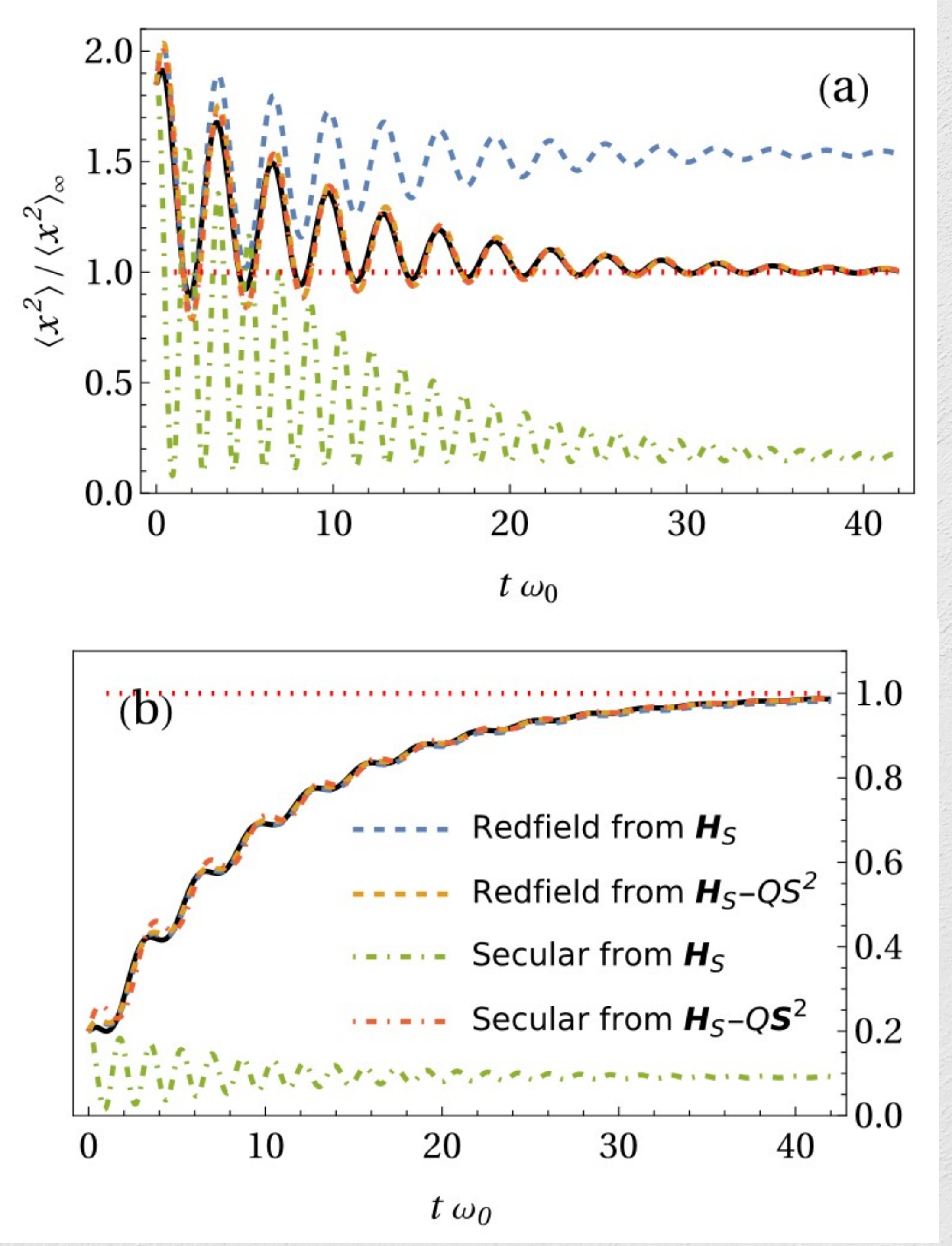
'reorganised' master equation

$$\frac{d\boldsymbol{\varrho}_S}{dt} = -i[\boldsymbol{H}_R + \boldsymbol{\Delta}^{(\gamma)}_{\boldsymbol{H}_R}, \boldsymbol{\varrho}_S] + \mathcal{R}^{(\gamma)}_{\boldsymbol{H}_R}\,\boldsymbol{\varrho}_S$$

secular
approximation

$$\frac{d\boldsymbol{\varrho}_S}{dt} = -i[\boldsymbol{H}_R, \boldsymbol{\varrho}_S] + \mathcal{D}_{\boldsymbol{H}_R}\,\boldsymbol{\varrho}_S$$

$$\boldsymbol{\varrho}_S(t \to \infty) \propto e^{-\beta\,(\boldsymbol{H}_S - Q\,\boldsymbol{S}^2)}$$


(a)
$\langle x^2 \rangle / \langle x^2 \rangle_\infty$
2.0
1.5
1.0
0.5
0.0
0
10
20
30
40
$t\,\omega_0$
(b)
1.0
0.8
0.6
0.4
0.2
0.0
Redfield from $\boldsymbol{H}_S$
Redfield from $\boldsymbol{H}_S$–QS^2
Secular from $\boldsymbol{H}_S$
Secular from $\boldsymbol{H}_S$–$Q\boldsymbol{S}^2$
0
10
20
30
40
$t\,\omega_0$

CONCLUSIONS

The common knowledge in open quantum systems applies only in the adiabatic limit and so long as the reorganisation energy is small.

Fixing a master equation so that it approaches the correct steady state tends to improve precision even during the transient dynamics.

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