Dissipative Quantum Systems from a Nonequilibrium Thermodynamicist's Perspective

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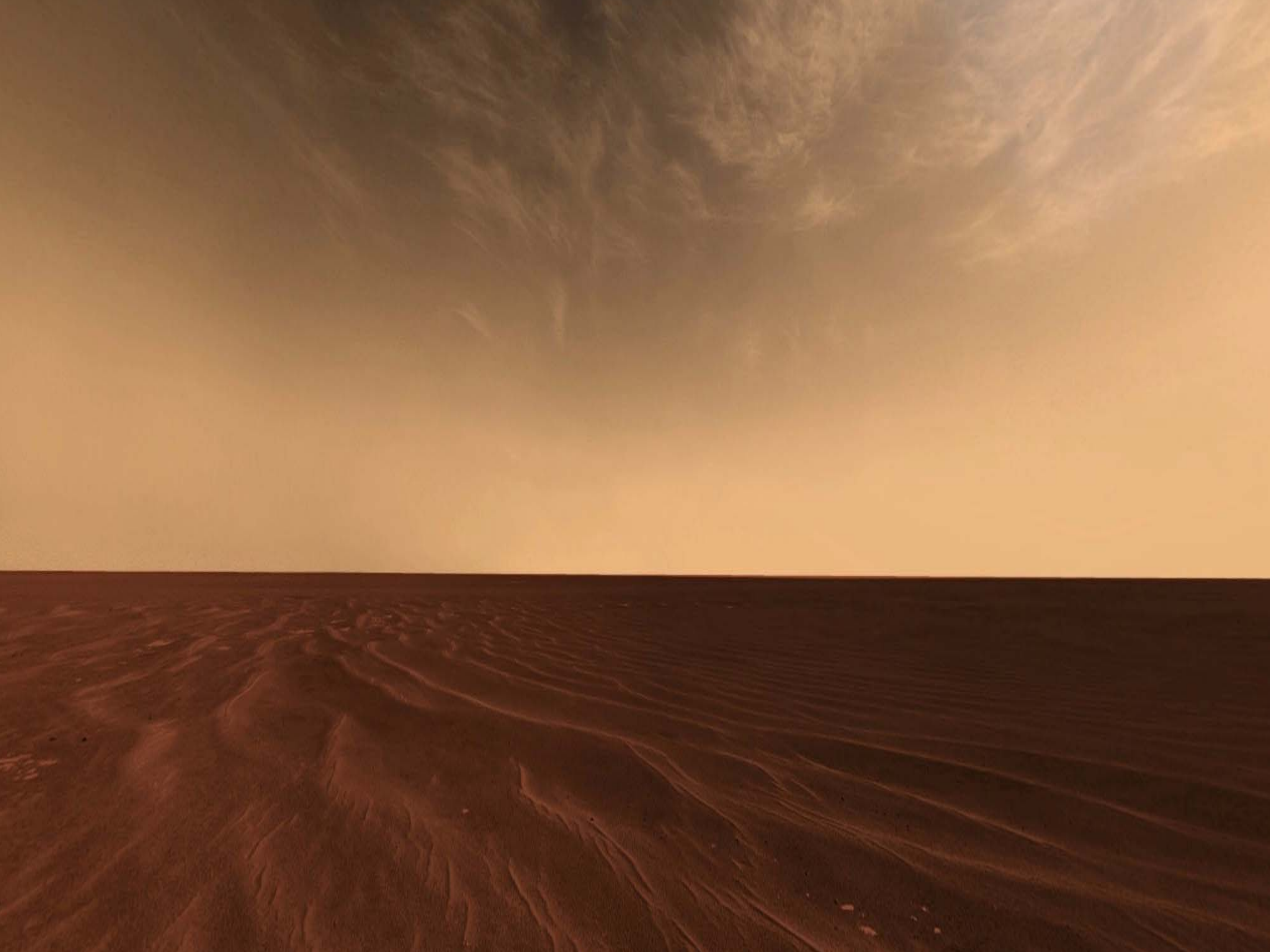
Outline

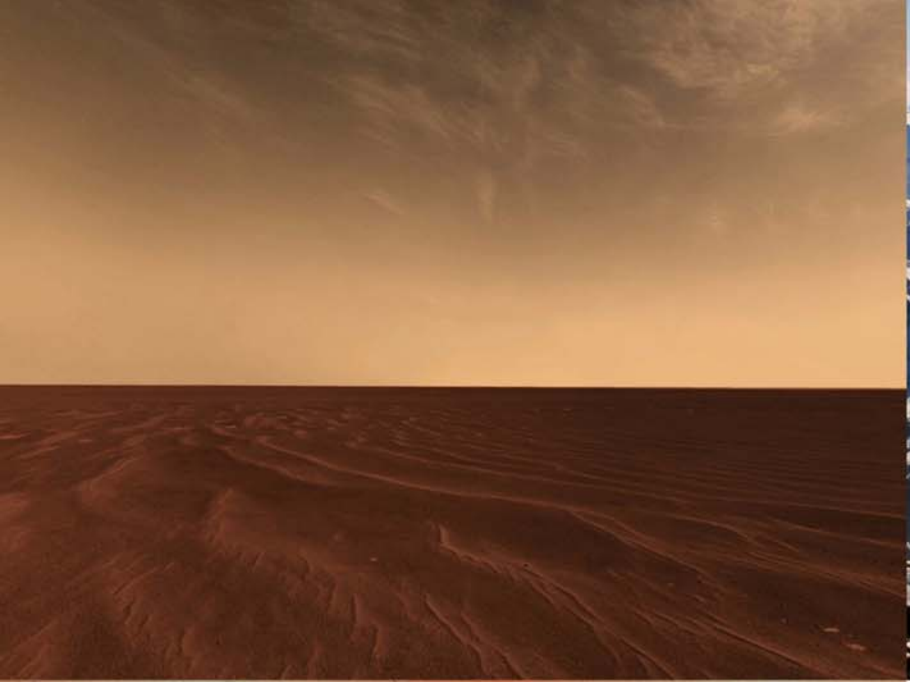
Geometry of classical nonequilibrium thermodynamics

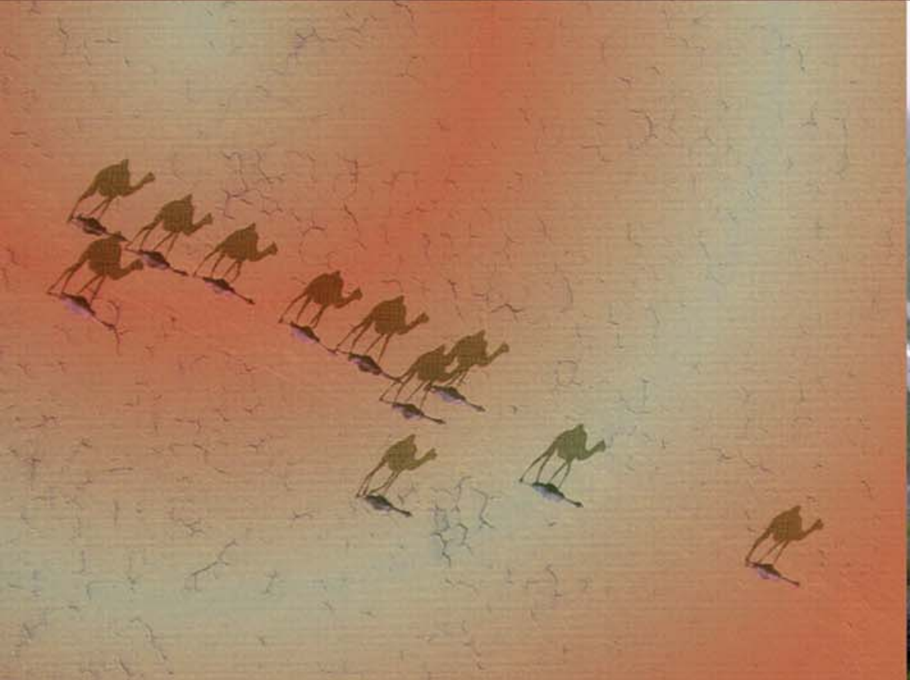
Geometry of dissipative quantum systems

Thermodynamic quantum master equation: Examples

Stochastic simulation techniques








GENERIC Structure

General equation for the nonequilibrium reversible-irreversible coupling

$$\frac{dA}{dt} = \{A, H\} + [A, S]$$

$H(x)$ energy

$S(x)$ entropy

Poisson bracket

$\{A,B\}$ antisymmetric,
Jacobi identity

$$\{A, S\} = 0$$

Dissipative bracket

$[A,B]$ Onsager/Casimir symmetric,
positive-semidefinite

$$[A, H] = 0$$

Physics of the Dissipative Bracket

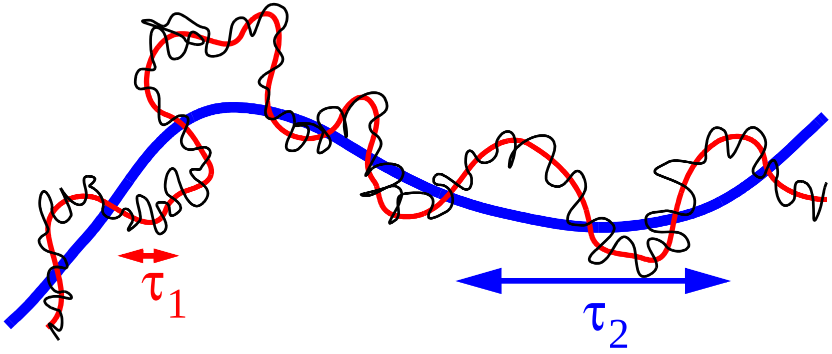
$$\frac{dS}{dt} = [S, S]$$

Frictional properties are related to time-dependent fluctuations:

cf. $D = \frac{1}{2\Delta t}\langle(\Delta x)^2\rangle$

Einstein

$$[A, B] = \frac{1}{2k_B\tau}\langle\Delta_\tau A^f\,\Delta_\tau B^f\rangle$$



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Dictionary: Quantum Subsystem & Environment

object	**quantum subsystem**	**classical environment**	**total**
state	statistical operator ρ	list of variables x	$(\rho \;\; x)$
observable	self-adjoint operator A	function A_e	$\tilde{A} = (A \;\; A_e)$
evaluation in state	$\langle A \rangle_\rho = \mathrm{tr}(A\rho)$	$A_{e,x} = A_e(x)$	$\bar{A} = \langle A \rangle_\rho + A_{e,x}$
energy	H	H_e	$\tilde{H} = (H \;\; H_e)$
entropy	$S = -k_B \ln \rho$	S_e	$\tilde{S} = (S \;\; S_e)$
Poisson bracket	$(A, B) = \frac{1}{i\hbar}[A, B]$	$\{A_e, B_e\}$	

GENERIC: Geometric Generalization

$$\frac{d\bar{A}}{dt} = \mathcal{P}(\tilde{A}, \tilde{H}) + \mathcal{D}(\tilde{A}, \tilde{S})$$

$$\mathcal{P}(\tilde{A}, \tilde{B}) = \{A_e, B_e\}_x + \langle (A, B) \rangle_\rho$$

coupling bracket(s)

coupling operator(s)

$$\mathcal{D}(\tilde{A}, \tilde{B}) = [A_e, B_e]_x + [H_e, H_e]_x^Q \langle (A, Q);(B, Q) \rangle_\rho$$

$$-[A_e, H_e]_x^Q \langle (H, Q);(B, Q) \rangle_\rho - [H_e, B_e]_x^Q \langle (A, Q);(H, Q) \rangle_\rho + [A_e, B_e]_x^Q \langle (H, Q);(H, Q) \rangle_\rho$$

GENERIC: Geometric Generalization

$$\frac{d\bar{A}}{dt} = \mathcal{P}(\tilde{A}, \tilde{H}) + \mathcal{D}(\tilde{A}, \tilde{S})$$

$$\mathcal{P}(\tilde{A}, \tilde{B}) = \{A_e, B_e\}_x + \langle (A, B) \rangle_\rho$$

$$\mathcal{D}(\tilde{A}, \tilde{B}) = [A_e, B_e]_x + [H_e, H_e]_x^Q \langle (A, Q);(B, Q) \rangle_\rho$$

coupling bracket(s)

coupling operator(s)

Canonical correlations as new geometric object for quantum dissipation:

$$\langle A;B \rangle_\rho = \int_0^1 \mathrm{tr}(\rho^\lambda A \rho^{1-\lambda} B) d\lambda = \mathrm{tr}(A_\rho B)$$

$$(\rho, A) = (\ln\rho, A_\rho)$$

$$A_\rho = \int_0^1 \rho^\lambda A \rho^{1-\lambda} d\lambda = \frac{1}{2}\left(A\rho + \rho A - \int_0^1 [\rho^\lambda, [\rho^{1-\lambda}, A]] d\lambda\right)$$

Nonlinear Thermodynamic Quantum Master Equation

Quantum subsystem:

$$\frac{d\rho}{dt} = \frac{i}{\hbar}[\rho, H] - \frac{1}{k_B}\sum_j [H_e, S_e]_x^j \, [Q_j, [Q_j, H]_\rho] - \sum_j [H_e, H_e]_x^j \, [Q_j, [Q_j, \rho]]$$

Heat bath: *H. Grabert,*
Z. Phys. B 49 (1982) 161

Quantum regression hypothesis:

$$\frac{d\rho}{dt} = -i\mathcal{L}\rho$$

Heisenberg picture $\Rightarrow$ $\langle [A(t), B] \rangle_\rho = \mathrm{tr}(A e^{-i\mathcal{L}t}[B, \rho])$

fluctuation-dissipation theorem $\Rightarrow$ $\langle [A(t), B] \rangle_\rho = \frac{\hbar}{kT_e}\mathrm{tr}(A e^{-i\mathcal{L}t}\mathcal{L}B_\rho)$

Nonlinear Thermodynamic Quantum Master Equation

Quantum subsystem:

Q_j itself is <u>not</u> affected by its own dissipation!

$$\frac{d\rho}{dt} = \frac{i}{\hbar}[\rho, H] - \frac{1}{k_B}\sum_j [H_e, S_e]_x^j \, [Q_j, [Q_j, H]_\rho] - \sum_j [H_e, H_e]_x^j \, [Q_j, [Q_j, \rho]]$$

Heat bath: *H. Grabert, Z. Phys. B 49 (1982) 161*

for $T_e [H_e, S_e]_{eq}^j = [H_e, H_e]_{eq}^j$: $\rho \propto \exp\left\{-\frac{H}{k_B T_e}\right\}$

Classical environment:

$$\frac{dA_{e,x}}{dt} = \{A_e, H_e\}_x + [A_e, S_e]_x - \frac{1}{k_B}\sum_j [A_e, S_e]_x^j \, \langle [Q_j, H];[Q_j, H]\rangle_\rho + \sum_j [A_e, H_e]_x^j \, \langle [Q_j, [Q_j, H]]\rangle_\rho$$

ETH Polymer Physics

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Particle in a Potential: Notation

Q position

P momentum

$V(Q)$ potential

$$[Q, P] = i\hbar$$

coupling bracket

$x = H_e, \quad S_e(H_e)$

$$[A_e, B_e]^Q = \frac{dA_e}{dH_e} \frac{k_B T_e \zeta}{\hbar^2} \frac{dB_e}{dH_e}$$

coupling operator

Q

Particle in a Potential: Results

$$\frac{d\langle Q\rangle_\rho}{dt} = \frac{\langle P\rangle_\rho}{m} \qquad \frac{d\langle P\rangle_\rho}{dt} = -\langle V'(Q)\rangle_\rho - \frac{\zeta}{m}\langle P\rangle_\rho$$

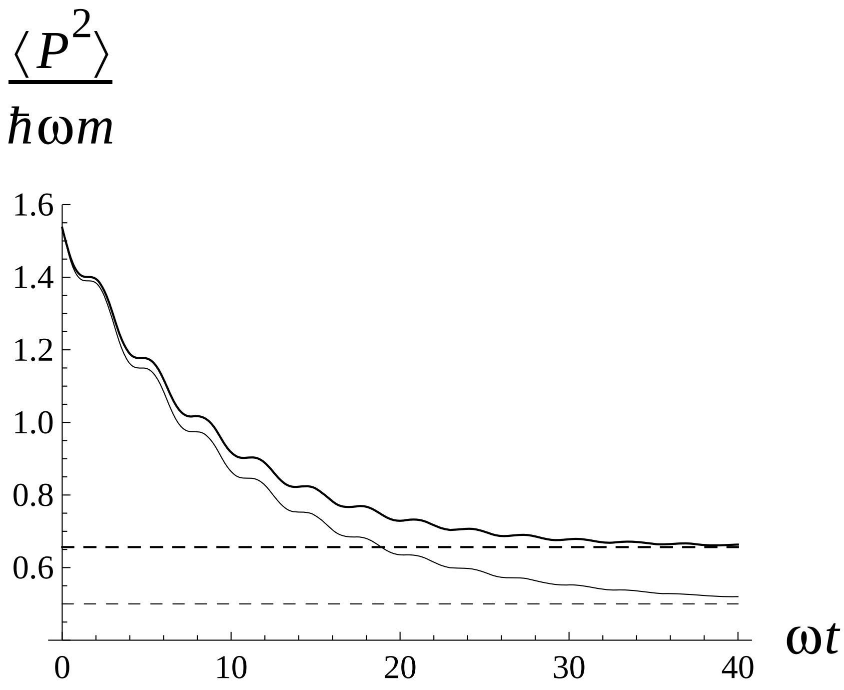
Ehrenfest & Caldeira-Leggett equation

$$\frac{d\langle Q^2\rangle_\rho}{dt} = \frac{1}{m}\langle QP + PQ\rangle_\rho$$

$$\frac{d\langle QP + PQ\rangle_\rho}{dt} = \frac{2}{m}\langle P^2\rangle_\rho - 2\langle QV'(Q)\rangle_\rho - 2\frac{\zeta}{m}\langle Q;P\rangle_\rho$$

$$\frac{d\langle P^2\rangle_\rho}{dt} = -\langle PV'(Q) + V'(Q)P\rangle_\rho - 2\frac{\zeta}{m}\langle P;P\rangle_\rho + 2k_B T_e \zeta$$

Particle in a Potential: Harmonic Oscillator



initially: $k_B T_e = \frac{3}{2}\hbar\omega$

quench: $k_B T_e = \frac{1}{2}\hbar\omega$

Two-Level Systems: Notation

$$A = \mathcal{O}(\alpha, \boldsymbol{a}) = \frac{1}{2}(\alpha I + a_1\sigma_1 + a_2\sigma_2 + a_3\sigma_3)$$

Pauli matrices

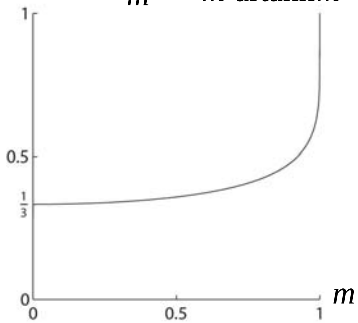
$$\rho = \mathcal{O}(1, \boldsymbol{m})$$

$$H = \frac{1}{2}\hbar\omega\,\sigma_3$$

$$[A, [A, B]] = \mathcal{O}(0, [a^2 1 - \boldsymbol{aa}] \cdot \boldsymbol{b})$$

$$\int_0^1 [\rho^{\lambda}, [\rho^{1-\lambda}, A]]d\lambda = \mu(m)\ \mathcal{O}(0, [m^2 1 - \boldsymbol{mm}] \cdot \boldsymbol{a})$$

$$\mu(m) = \frac{1}{m^2} - \frac{1}{m\ \mathrm{artanh} m}$$



coupling brackets

$$x = H_e, \quad S_e(H_e)$$

$$[A_e, B_e]^j = \frac{dA_e}{dH_e}\gamma_0\frac{k_B T_e}{\hbar\omega}\frac{dB_e}{dH_e}$$

coupling operators

$$\sigma_1, \sigma_2 \quad (\sigma_3)$$

Two-Level Systems: Results

$$\frac{d\boldsymbol{m}}{dt} = \omega \boldsymbol{q}_3 \times \boldsymbol{m} - \gamma_0 \frac{2k_B T_e}{\hbar\omega} \boldsymbol{R} \cdot \boldsymbol{m} - \gamma_0 \boldsymbol{q}_3 + \gamma_0 \frac{\mu}{2} (m^2 1 + \boldsymbol{m}\boldsymbol{m}) \cdot \boldsymbol{q}_3$$

$$\boldsymbol{R} = \begin{bmatrix} 1/2 & 0 & 0 \\ 0 & 1/2 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\boldsymbol{m}_{eq} = -\boldsymbol{q}_3 \tanh\left(\frac{\hbar\omega}{2k_B T_e}\right)$$

system stays
in Bloch sphere: $m \leq 1$

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Stochastic Simulations

inspired by *H.-P. Breuer and F. Petruccione, The Theory of Open Quantum Systems (2002)*

jump operator $\tilde{Q} = \alpha(Q + \beta[Q, H]_\rho \rho^{-1})$

quantum jumps $\psi \to \tilde{Q}\psi$ with rate γ

deterministic evolution $\frac{d\psi}{dt} = -\frac{i}{\hbar} H\psi + \Lambda\psi$

$\rho = \mathrm{E}(|\psi\rangle\langle\psi|)$ $\frac{d\rho}{dt} = \frac{i}{\hbar}[\rho, H] + \Lambda\rho + \rho\Lambda^+ + \gamma(\tilde{Q}\rho\tilde{Q}^+ - \rho)$

averages required!
normalization preserved on average only!
warning: variance of normalization!

Take-Home Messages

- There exists a (beautiful) *geometric formulation* of classical *nonequilibrium thermodynamics* (far away from equilibrium!)
- The generalization to *dissipative quantum systems* by Dirac's *method of classical analogy* is supported nicely by the geometric formulation
- We obtain a (beautiful) nonlinear *quantum master equation* (plus an equation for the environment)
- *Thermodynamic nonlinearity* improves the behavior of solutions
- *Stochastic simulation techniques* are available (and tested)
- Environments and couplings of enormous *generality* can be handled, including open environments

Outlook

quantum field theory

Further Reading

hco, Phys. Rev. A 82, 052119 (2010) [11 pages]