Quantum Brownian Motion: Facts, debatable issues and unsolved issues

Peter Hänggi and Gert Ingold

Brownian Motion 2025, EPFL, Lausanne, CH

Theory of Brownian motion

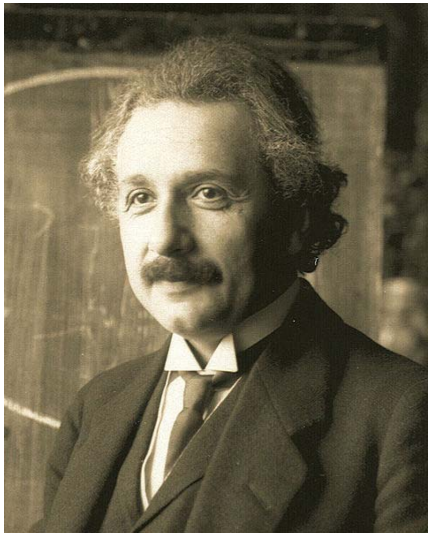
W. Sutherland (1858-1911)

Source: www.theage.com.au

$$D = \frac{RT}{6\pi\eta a C}$$

Phil. Mag. **9**, 781 (1905)

A. Einstein (1879-1955)



Source: wikipedia.org

$$\langle x^2(t) \rangle = 2Dt$$

$$D = \frac{RT}{N} \frac{1}{6\pi k P}$$

Ann. Phys. **17**, 549 (1905)

M. Smoluchowski (1872-1917)

Source: wikipedia.org

$$D = \frac{32}{243} \frac{mc^2}{\pi\mu R}$$

Ann. Phys. **21**, 756 (1906)

Dynamics of Open Quantum Systems

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QUANTUM DISSIPATION

$$L = \frac{1}{2} m_0 e^{\gamma t} \dot{x}^2 - \frac{1}{2} m_0 e^{\gamma t} \omega_0^2 x^2$$

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}} = \frac{d}{dt} m_0 e^{\gamma t} \dot{x} = m_0 e^{\gamma t} \ddot{x} + m_0 e^{\gamma t} \gamma \dot{x}$$

$$-\frac{\partial L}{\partial x} = m_0 e^{\gamma t} \omega_0^2 x$$

$$\Rightarrow \cancel{e^{\gamma t}} \left[m_0 \ddot{x} + m_0 \gamma \dot{x} + m_0 \omega_0^2 x \right] = 0$$

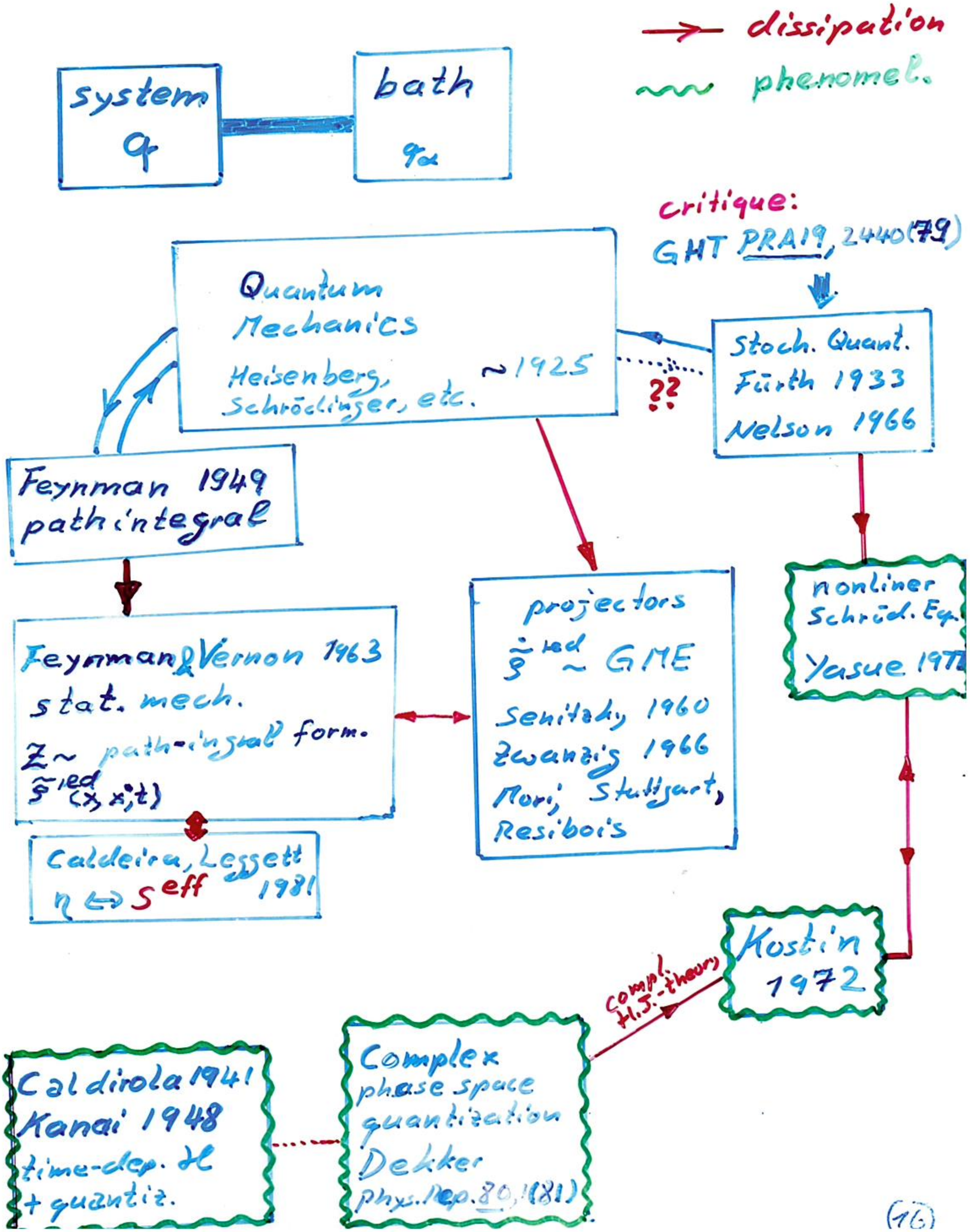
$$\text{QM: } L \rightarrow H = \frac{p^2}{2m_0} e^{-\gamma t} + \frac{1}{2} m_0 e^{\gamma t} \omega_0^2 x^2$$

$$\text{¡} \quad [\Delta x, \Delta p] = i\hbar e^{-\gamma t}$$

W. E. Brittin, Phys. Rev. 77, 396 (1950)
Chung-In Um, K. H. Yeon, T. F. George, Phys. Rep. 362, 63ff (2002) (129 pages!)

Quantum Dissipation

How ??



real world quantum dissipation

- do not rely ("trust") more or less inspired guesswork

- do the full Q.M. in the universe

  do the hard work for a realistic laboratory set-up, – account for noise!

  Caldeira & Leggett, Grabert, Weiss, Hänggi, Schmid, Larkin, ...

- extract the relevant information by integration over bath degrees of freedom

ISSN 0 370-1573

PHYSICS REPORTS

A Review Section of Physics Letters

QUANTUM BROWNIAN MOTION: THE FUNCTIONAL INTEGRAL APPROACH

Hermann GRABERT, Peter SCHRAMM and Gert-Ludwig INGOLD

Volume 168 Number 3

October 1988

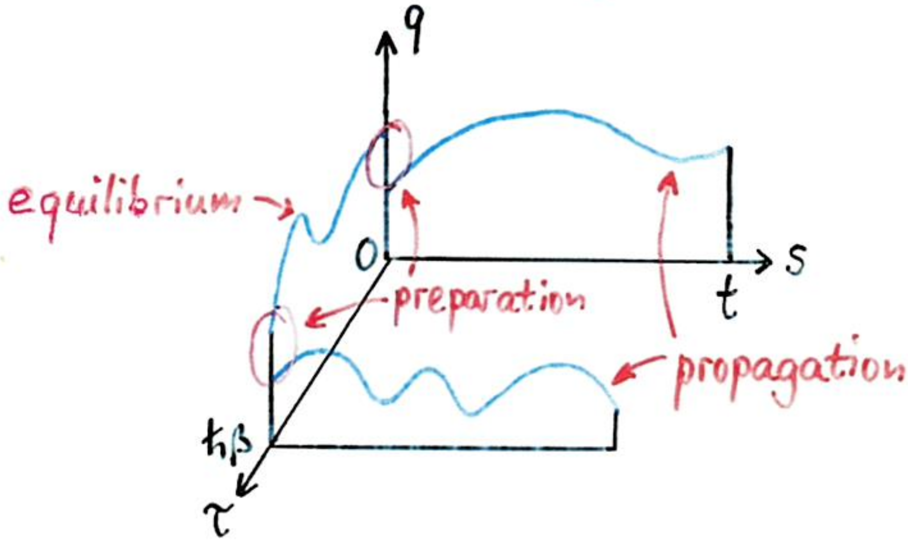
PRPLCM 168(3) 115–207 (1988)

NORTH-HOLLAND · AMSTERDAM

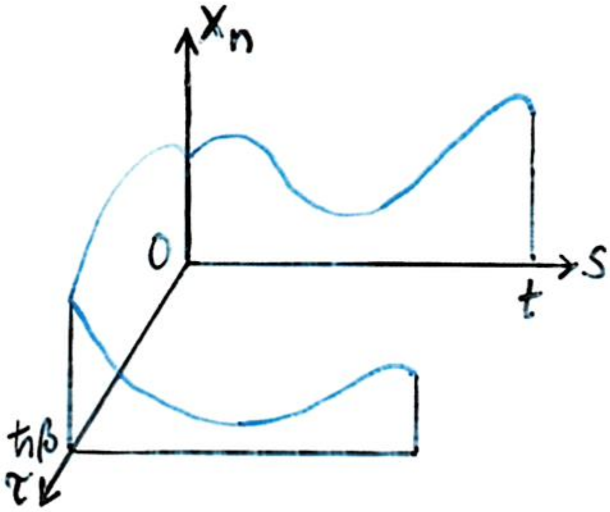
density matrix of system + heat bath:

$$W(t) = e^{-\frac{i}{\hbar}Ht} \sum_j \left(O_j \, e^{-\beta H} \, O_j' \right) e^{\frac{i}{\hbar}Ht}$$

use functional integrals

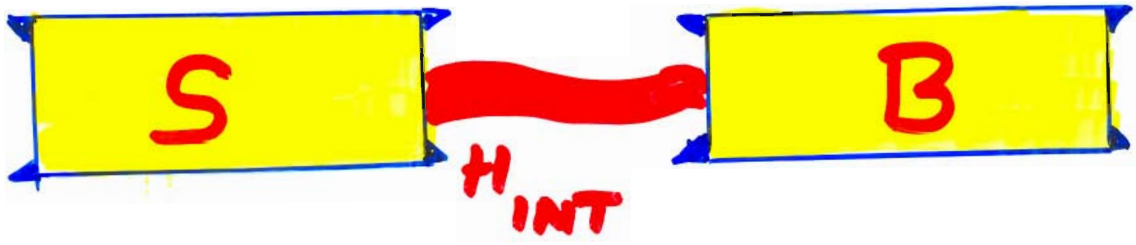


system



heat bath

QUANTUM NOISE



NO QUANTUM EQ.-PARTITION-TH.

FEYNMAN-PATH-INT.

$\Updownarrow$

QUANTUM LANG.-EQ.

$\Updownarrow$

GME

$\Updownarrow$

STOCH.-L.-v.N.-EQ.

$$\rho := |\psi_1(t)\rangle\langle\psi_2(t)| \; ; \; \mu := \frac{2}{\pi}\int_0^\infty d\omega \, \frac{J(\omega)}{\omega}$$

$$i\hbar\dot{\rho} = [H_0, \rho] + \frac{\mu}{2}[x^2, \rho] - \xi(t)[x, \rho] - \frac{\hbar}{2}\nu(t)\{x, \rho\}_+$$

COMPLEX VALUED NOISE

$$\langle \xi(t)\xi(t')\rangle = \mathrm{Re}\, L(t-t') \; ; \; \langle \xi(t)\nu(t')\rangle = \frac{2i}{\hbar}\,\theta(t-t')\,\mathrm{Im}\, L(t-t')$$

$$\langle \nu(t)\nu(t')\rangle = 0$$

PHYSICAL REVIEW A **69**, 052109 (2004)

Is the dynamics of open quantum systems always linear?

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(Received 1 December 2003; published 17 May 2004)

We study the influence of the preparation of an open quantum system on its reduced time evolution. In contrast to the frequently considered case of an initial preparation where the total density matrix factorizes into a product of a system density matrix and a bath density matrix the time evolution generally is no longer governed by a linear map nor is this map affine. Put differently, the evolution is truly nonlinear and cannot be cast into the form of a linear map plus a term that is independent of the initial density matrix of the open quantum system. As a consequence, the inhomogeneity that emerges in formally exact generalized master equations is in fact a nonlinear term that vanishes for a factorizing initial state. The general results are elucidated with the example of two interacting spins prepared at thermal equilibrium with one spin subjected to an external field. The second spin represents the environment. The field allows the preparation of mixed density matrices of the first spin that can be represented as a convex combination of two limiting pure states, i.e., the preparable reduced density matrices make up a convex set. Moreover, the map from these reduced density matrices onto the corresponding density matrices of the total system is affine only for vanishing coupling between the spins. In general, the set of the accessible total density matrices is nonconvex.

microscopic approach

$$H^{total} = \underbrace{\frac{1}{2} M \dot{q}^2 + U(q)}_{\text{system}}$$

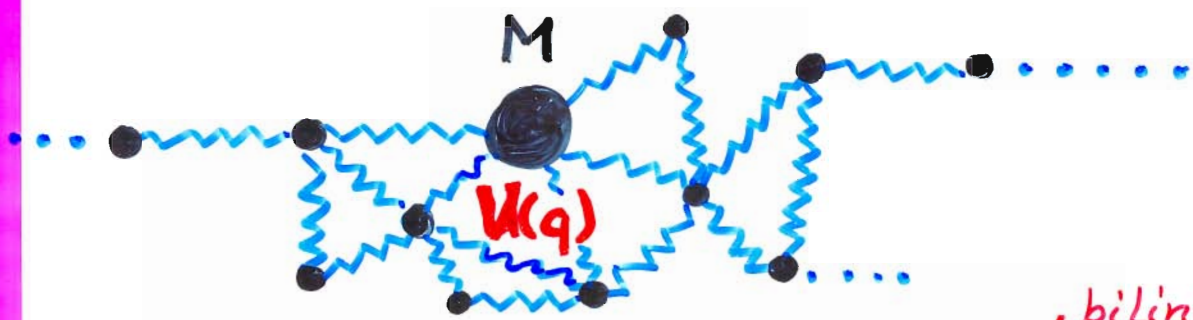
$$+ \underbrace{\frac{1}{2} \sum_\alpha m_\alpha \dot{q}_\alpha^2 + \sum_\alpha m_\alpha \omega_\alpha^2 q_\alpha^2}_{\text{(harmonic) bath}}$$

$$+ \underbrace{q \sum_\alpha c_\alpha q_\alpha}_{\text{linear coupling}}$$

$$+ \underbrace{q^2 \sum_\alpha \frac{c_\alpha^2}{2 m_\alpha \omega_\alpha^2}}_{\text{compensation of frequency shift}}$$

- path integral approach to density matrix at temperature T
- trace out environment

dissipation



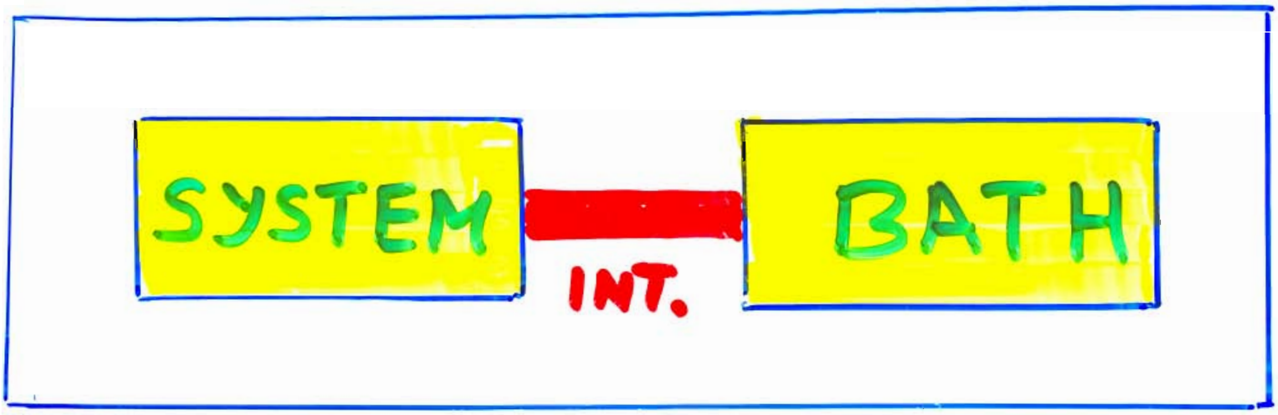
bilinear

$$H^T = H_{system} + H_{bath} + H_{Int}$$

$$\ddot{q} = -\frac{1}{M}\frac{\partial U}{\partial q} - \int_0^t \gamma(t-s)\,\dot{q}(s)\,ds$$

$$S_E = S_{rev.\ motion} + S_{dissipation}\ (\text{nonlocal})$$

QUANTUM L.-EQ.



$$|0\rangle_{S+B} \neq |0\rangle_S \, |0\rangle_B$$

↳ **DECOHERENCE AT $T = 0$**

$$\mathbb{H}_{S+B} = \mathbb{H}_S + \mathbb{H}_{S-B} + \mathbb{H}_B$$

$$= \frac{p^2}{2m} + V(x) + \sum_\alpha \left[\frac{p_\alpha^2}{2m_\alpha} + \frac{m_\alpha \omega_\alpha^2}{2} \left(q_\alpha - \frac{c_\alpha}{m_\alpha \omega_\alpha^2} x \right)^2 \right]$$

$$¡\ \rho_S \neq Z^{-1} \exp\left(-\frac{\mathbb{H}_S}{kT} \right) !$$

$$\rho_{Total} = \rho_{S+B} = Z^{-1} \exp\left(-\frac{\mathbb{H}_{S+B}}{kT} \right)$$

Q L E

$$i\hbar\,\dot{\mathbb{O}} = [\mathbb{O}, \mathbb{H}_T]$$

$$m\ddot{x} + m\int_0^t ds\,\gamma(t-s)\,\dot{x}(s) + \frac{\partial V(x)}{\partial x} = \eta(t) \underbrace{- m\gamma(t-0)\,x(0)}_{\text{INITIAL SLIP}}$$

$$!\;\gamma(t-s) = \frac{1}{m}\sum_\alpha \frac{c_\alpha^2}{m_\alpha \omega_\alpha^2}\cos(\omega_\alpha(t-s))$$

$$= \gamma(s-t)$$

$$\eta(t) = \sum_\alpha c_\alpha \left[q_\alpha(0)\cos(\omega_\alpha t) + \frac{p_\alpha}{m_\alpha \omega_\alpha}\sin(\omega_\alpha t) \right]$$

- $[\eta(t), \eta(s)] = -i\hbar \sum_\alpha \frac{c_\alpha^2}{m_\alpha \omega_\alpha} \sin(\omega_\alpha (t-s))$

$\neq 0$

$$\rho_B = Z^{-1} \exp\left\{-\beta\left[\sum_\alpha \left(\frac{p_\alpha^2}{2m_\alpha} + \frac{m\omega_\alpha^2}{2} q_\alpha^2\right)\right]\right\}$$

- $\langle \eta(t) \rangle_{\rho_B} = 0$

- $\frac{1}{2}\langle \eta(t)\eta(s) + \eta(s)\eta(t) \rangle = C(t-s)$

$$= C(\tau) = \frac{\hbar}{2} \sum_\alpha \frac{c_\alpha^2}{m_\alpha \omega_\alpha} \coth\left(\frac{\hbar\omega_\alpha}{2kT}\right) \cos(\omega_\alpha \tau)$$

$$\xrightarrow{kT \gg \hbar\omega_\alpha} kT\gamma(\tau)$$

REMARKS

1.

QLE OPERATES IN FULL HILBERT SPACE OF $S \oplus B$

2.

$$\hat{\gamma}(z) = \int_0^\infty e^{izt}\gamma(t)\,dt = \frac{i}{2m}\sum_\alpha \frac{c_\alpha^2}{m_\alpha\omega_\alpha^2}\left[\frac{1}{z-\omega_\alpha} + \frac{1}{z+\omega_\alpha}\right]$$

$\mathrm{Im}\, z > 0$

$$\frac{1}{x+i0^+} = P\left(\frac{1}{x}\right) - i\pi\delta(x)$$

$$\mathrm{Re}\,\hat{\gamma}(z = \omega + i0^+) = \frac{\pi}{2m}\sum_\alpha \frac{c_\alpha^2}{m_\alpha\omega_\alpha^2}\left[\delta(\omega-\omega_\alpha) + \delta(\omega+\omega_\alpha)\right]$$

$$\boxed{C(\tau) = \frac{m}{\pi}\int_0^\infty d\omega\, \mathrm{Re}\,\hat{\gamma}(\omega + i0^+)\cos(\omega\tau) \times \coth\left(\frac{\hbar\omega}{2kT}\right)}$$

3. with $\xi(t) = \eta(t) - m\gamma(t)\,x(0)$

$$\hat{\rho}_B = Z^{-1}\exp -\beta\left[\sum_\alpha\left(\frac{p_\alpha^2}{2m_\alpha} + \frac{m_\alpha\omega_\alpha^2}{2}\left(q_\alpha - \frac{c_\alpha}{m_\alpha\omega_\alpha^2}x\right)^2\right)\right]$$

$$\Rightarrow \langle \xi(t)\rangle_{\hat{\rho}} = 0$$

$$\frac{1}{2}\langle \xi(\tau)\xi(0) + \xi(0)\xi(t)\rangle_{\hat{\rho}} = C(\tau)$$

$\boxed{4.}$ ¿ DEPHASING AT $T=0$!

$$\langle X(0)\,\xi(t)\rangle_{\hat{\rho}} \neq 0$$

$$\langle \mathbb{H}_{INT}\rangle_{\hat{\rho}} \neq 0$$

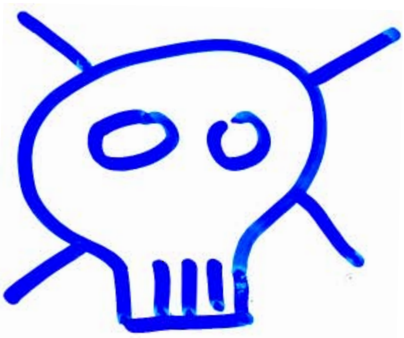
$\boxed{5.}$

$\xi(t) \longrightarrow$ C-NOISE $\xi(t)$

WITH CORRELATION

$C(\tau)$

IS INCONSISTENT



PITFALLS

MARKOV MASTER EQ

$$\frac{d}{dt}\rho = -\frac{i}{\hbar} L \rho - \Gamma\rho + I(t)$$

BLOCH-REDFIELD

i.g. NO DET. BALANCE

ROTATING WAVE APPROX.

(LINDBLAD: DAVIES-APPROX.)

DET. BALANCE ✓ O.K.

BUT

- WRONG EHRENFEST EQ.
- NO FDT
- NO KMS-COND. $\langle u(t)\, v\rangle_\beta = \langle v\, u(t+i\hbar\beta)\rangle_\beta$

TIME REVERSAL

$$m\ddot{x} + m\int_0^t ds\, \gamma(t-s)\,\dot{x}(s) + \frac{\partial V}{\partial x} = -m\gamma(t)\,x(0) + \xi(t)$$

$$t \to -t \quad \Rightarrow y = x(-t)$$

$$y(0) = x(0)$$
$$q_\alpha(0) = q_\alpha(0)$$
$$p_\alpha(0) = -p_\alpha(0)$$

WITH $\dot{y}(t) = \frac{d}{dt} x(-t) = -\dot{x}(-t)$

$$\ddot{y}(t) = \ddot{x}(-t)$$
$$\dot{x}(s) = -\dot{y}(-s)$$

$$m\ddot{y}(t) + m\int_0^{-t} ds\, \gamma(-s-t)\left[-\dot{y}(-s)\right] + \frac{\partial V}{\partial y} = -m\gamma(t)\,x(0) + \xi(t)$$

$$\tau = -s\ ;\ ds = -d\tau$$

$$\gamma(\tau - t) = \gamma(t-\tau)$$

$$\Rightarrow\ m\ddot{y}(t) + m\int_0^t d\tau\, \gamma(t-\tau)\,\dot{y}(\tau) + \frac{\partial V}{\partial y} = -m\gamma(t)\,y(0) + \xi(t)$$

OHMIC FRICTION: $\gamma(t-s) = 2\gamma\,\delta(t-s)$

$$m\ddot{x} = -\frac{\partial V}{\partial x} - m\gamma\dot{x}\begin{Bmatrix} 1;\ t>0 \\ -1;\ t<0 \end{Bmatrix} + \xi(t)$$

FREE QUANTUM Brownian MOTION

Using the path integral methodology in full phase space

of system + bath + interaction

$$\Rightarrow \quad H = \frac{p^2}{2M_0} + U(q)$$

$$+ \sum_{n=1}^{N\to\infty} \left[\frac{p_n^2}{2m_n} + \frac{1}{2} m_n \omega_n^2 \left(q_n - \frac{c_n q}{m_n \omega_n^2} \right)^2 \right]$$

spectral density

$$I(\omega) = \frac{\pi}{2} \sum_{n=1}^{N} \frac{c_n^2}{m_n \omega_n} \delta(\omega - \omega_n)$$

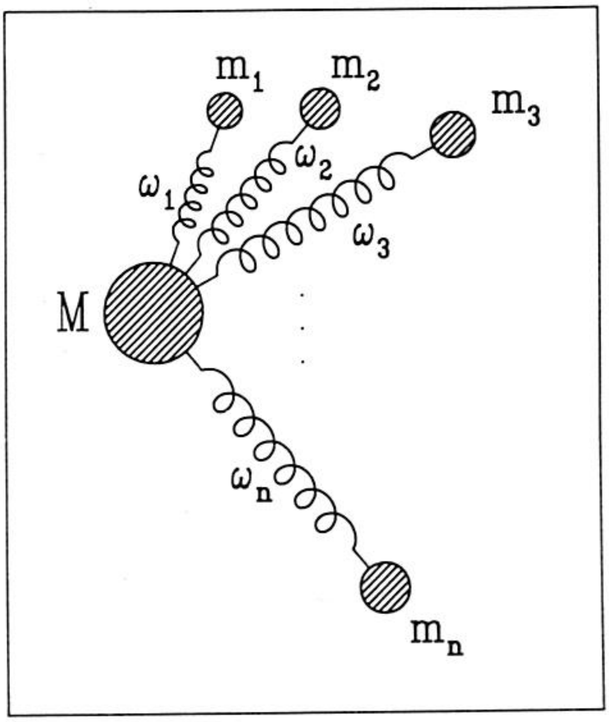
$$= M_0 \gamma \omega \quad \Leftrightarrow \text{ Ohmic dissipation}$$

"$-\gamma \dot{q}$"

$$= M g_\alpha \, \omega^\alpha \, H(\omega_c - \omega) \quad ; \alpha > 0$$

non-Ohmic

free Brownian Quantum motion



$$U(q) = 0$$

$$c_n = m_n \omega_n^2$$

$$H = \frac{p^2}{2M_0} + \sum_{n=1}^{N\to\infty} \left[\frac{p_n^2}{2m_n} + \frac{1}{2} m_n \omega_n^2 (q_n - q)^2 \right]$$

translationally invariant

"Free" displacement correlation fct.

$$Q^F(t) = \frac{1}{2}\left\{\langle [q(t)-q(0)]\,q(0)\rangle + \langle q(0)\,[q(t)-q(0)]\rangle\right\}$$

$$= \frac{1}{2}\left\{\langle q(t)q(0)\rangle - \langle q^2(0)\rangle + \langle q(0)q(t)\rangle - \langle q^2(0)\rangle\right\}$$

$$= \underbrace{\frac{1}{2}\left\{\langle q(t)q(0)\rangle + \langle q(0)q(t)\rangle\right\}}_{S'(t)} - \langle q^2(0)\rangle$$

diverges! for $\omega_0 \to 0$

$\propto k_BT/M\omega_0$

$$= \underbrace{S'(t) - \langle q^2\rangle_{eq}}_{\text{is regular}}$$

mean square displacement: $s(t)$

$$s(t) = \langle (q(t)-q(0))^2\rangle = \langle (q(t)-q(0))(q(t)-q(0))\rangle$$

$$= \langle q^2(t)\rangle + \langle q^2(0)\rangle - \langle q(t)q(0)\rangle - \langle q(0)q(t)\rangle$$

$$\boxed{s(t) = -2\,Q^F(t)} + \underbrace{\langle q^2(t)\rangle_{eq} + \langle q^2(0)\rangle_{eq} - 2\langle q^2(0)\rangle_{eq}}_{0}$$

at $T=0$ $\quad s(t) \xrightarrow{T\to 0} \equiv s_0(t)$ notation

Table 3

Asymptotic long-time dependence of the mean square displacement [$s_0(t)$ for $T=0$ and $s(t)$ for $T>0$] and the antisymmetrized part $A^{\mathrm{F}}(t)$ of the displacement correlation function in terms of the exponent α and the quantities defined in eqs. (11.19–11.23). The symmetrized part $Q^{\mathrm{F}}(t)$ of the displacement correlation function is given by $Q^{\mathrm{F}}(t)=-s(t)/2$

α	$s_0(t)$ $[T=0]$	$A^{\mathrm{F}}(t)$	$s(t)$ $[T>0]$
$0<\alpha<1$	$2q_\infty$		
$\alpha=1$	$2d_1\ln(t)\times[1+\mathrm{O}(\ln^{-1}(t))]$	$-(\alpha\hbar/2\mu_\alpha)t^{\alpha-1}\times[1+\mathrm{O}(t^{-1},t^{\alpha-2})]$	$2D_\alpha t^\alpha\times[1+\mathrm{O}(t^{-1},t^{\alpha-2})]$
$1<\alpha<2$	$2d_\alpha t^{\alpha-1}\times[1+\mathrm{O}(t^{\alpha-2})]$		
$\alpha=2$	$2d_2t/\ln^2(t)\times[1+\mathrm{O}(\ln^{-1}(t))]$	$-(\hbar/\mu_2)t/\ln(t)\times[1+\mathrm{O}(\ln^{-1}(t))]$	$2D_2t^2/\ln(t)\times[1+\mathrm{O}(\ln^{-1}(t))]$
$2<\alpha<3$	$2d_\alpha t^{3-\alpha}\times[1+\mathrm{O}(t^{2-\alpha})]$		
$\alpha=3$	$2d_3\ln(t)\times[1+\mathrm{O}(\ln^{-1}(t))]$	$-(\hbar/2M_r)t\times[1+\mathrm{O}(t^{-2},t^{2-\alpha})]$	$2(v_\beta^2/2)t^2\times[1+\mathrm{O}(t^{-2},t^{2-\alpha})]$
$3<\alpha$	constant		

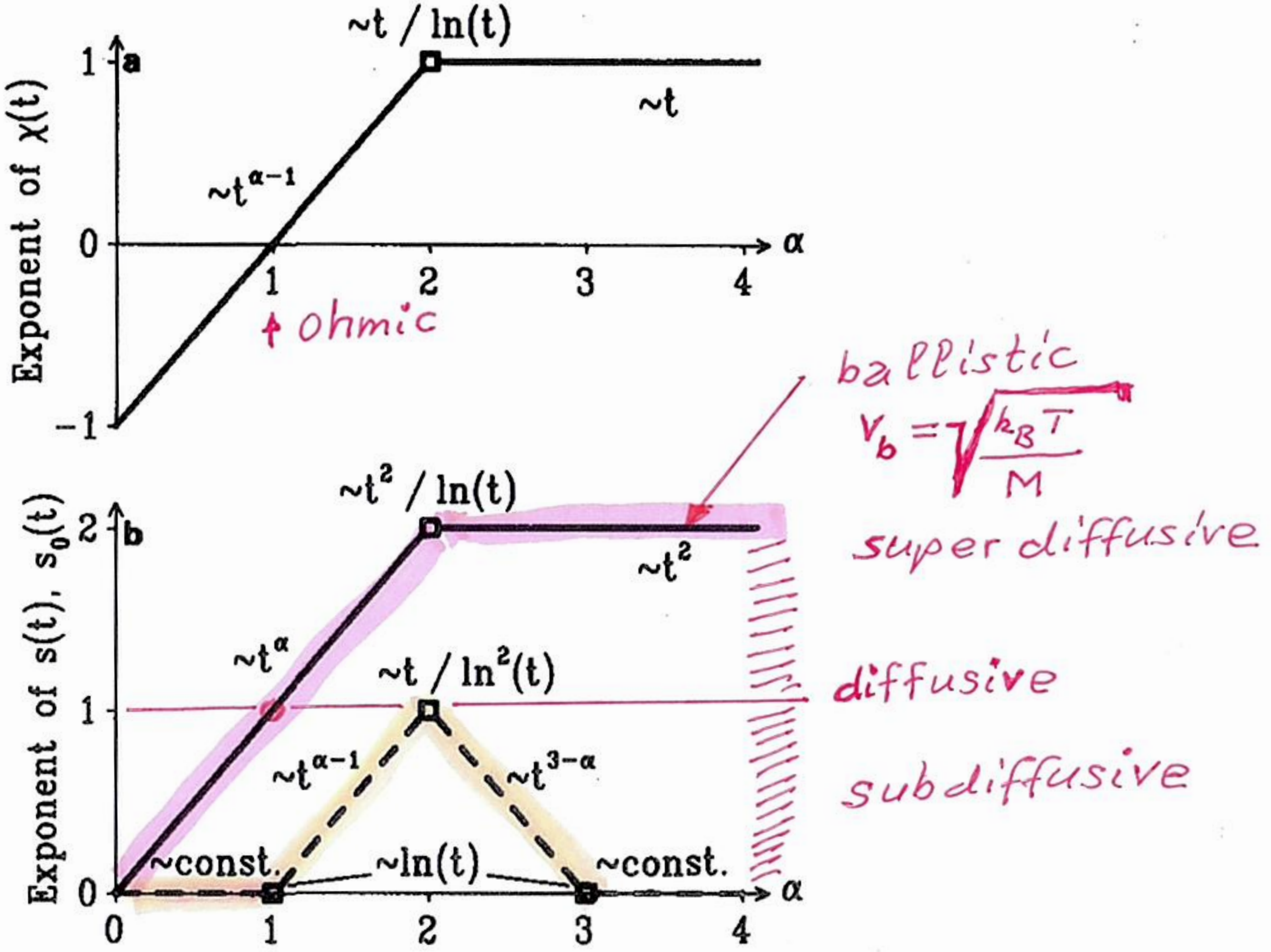


Fig. 7. (a) The exponent of the asymptotic time dependence of the response function $\chi(t)$ is shown as a function of the spectral exponent α. (b) The solid (dashed) line shows the exponent of the asymptotic time dependence of the mean square displacement $s(t)(s_0(t))$ for finite (zero) temperature as a function of the spectral exponent α.

SYNOPSIS

LINEAR RESPONSE THEORY & QUANTUM-FDT

$$\hat{H}(t) = \hat{H}_0 - \mathcal{F}(t)\hat{A} \quad ; \quad \varrho_\beta = Z^{-1}\exp(-\beta \hat{H}_0)$$

$$\langle \hat{B}(t)\rangle - \langle \hat{B}(t)\rangle_\beta = \langle \delta\hat{B}(t)\rangle = \int_{t_0}^{t} \chi_{BA}(t-s)\,\mathcal{F}(s)\,ds$$

KUBO: $$\chi_{BA}(\tau) = \Theta(\tau)\frac{i}{\hbar}\langle[\hat{B}(\tau), \hat{A}(0)]\rangle_\beta$$

$$= -\Theta(\tau)\int_0^\beta \langle \hat{A}(-i\hbar\lambda)\dot{\hat{B}}(\tau)\rangle_\beta\, d\lambda$$

classical limit $\rightarrow -\Theta(\tau)\beta\langle \dot{B}(\tau)A(0)\rangle_\beta$

$$\hat{B} = \hat{A} = \hat{q} \quad ; \quad \mathcal{F}(t) = A\cos\Omega t$$

$$\langle \delta\hat{q}(t)\rangle = P_1 e^{-i\Omega t} + P_{-1} e^{-i\Omega t}$$

$$P_{1,-1} = \frac{A}{2} e^{\mp i\Omega t}\chi(\pm\Omega)$$

QUANTUM – FDT

$$S_{BA}(\tau) = \frac{1}{2}\Big\langle \big(\hat{B}(t) - \langle \hat{B}\rangle_\beta\big)\big(\hat{A}(0) - \langle \hat{A}\rangle_\beta\big) + \big(\hat{A}(0) - \langle \hat{A}\rangle_\beta\big)\big(\hat{B}(\tau) - \langle \hat{B}\rangle_\beta\big)\Big\rangle_\beta$$

$$\chi_{BA}(\tau) = \chi'_{BA}(\tau) + i\,\chi''_{BA}(\tau)$$

$$\frac{1}{2}\left[\chi_{BA}(t) + \chi_{AB}(-t)\right] \qquad -\frac{i}{2}\left[\chi_{BA}(t) - \chi_{AB}(-t)\right]$$

$$\chi_{BA}(\omega) = \int_{\cancel{-\infty}\; 0}^{\infty} \chi_{BA}(t)\, e^{i\omega t}\, dt$$

$$\Rightarrow \quad \chi''_{BA}(\omega) = \frac{1}{\hbar}\tanh(\hbar\omega\beta/2)\, S_{BA}(\omega)$$

$$S_{BA}(\omega) = \hbar\coth(\hbar\omega\beta/2)\,\chi''_{BA}(\omega)$$

$$\xrightarrow{\hbar\omega\beta \ll 1} \; 2\,\chi''_{BA}(\omega)/(\beta\Omega)$$

<u>NOTE:</u> $\chi''_{BA}(\omega) = \frac{i}{2}\left[\chi^{*}_{AB}(\omega) - \chi_{BA}(\omega)\right]$

$\neq \mathrm{Im}\,\chi_{BA}(\omega)$; except $\hat{A} = \hat{B}$

$\hat{A} = \hat{B} = \hat{q}$: $$\underline{\underline{S_{qq}(\Omega) = \hbar\coth(\hbar\Omega\beta/2)\,\mathrm{Im}\,\chi_{qq}(\Omega)}}$$

EQ.-CURRENT NOISE

$\mathbb{A} = \mathbb{B}$ $\quad \mathbb{I} := \frac{d\mathbb{B}}{dt}$; $\langle \delta I(t) \rangle = \int_{-\infty}^{t} Z(t-s) F(s) ds$

$$Z(t-s=\tau) = \frac{d\chi(\tau)}{d\tau}$$

$$\chi''_{AA}(\omega) = \frac{1}{\omega} \operatorname{Im}\left(\frac{Z(\omega)}{i}\right) = -\frac{1}{\omega} \operatorname{Re} Z(\omega)$$

$$S_{II}(\omega) = -\omega^2 S_{BB}(\omega)$$

$$S_{II}(\omega) = (\hbar\omega) \coth\left(\frac{\hbar\omega}{2kT}\right) \operatorname{Re} Z(\omega)$$

$kT \gg \hbar\omega$: $S_{II}(\omega) \rightarrow 2kT \operatorname{Re} Z(\omega)$

$$\xrightarrow{\text{MARKOV}} \underline{2kT/R}$$

JOHNSON-NYQUIST (1928)

$kT \ll \hbar\omega \longrightarrow \hbar\omega \operatorname{Re} Z(\omega)$

quantum-zero point fluct.

$S_{II}(\omega=0) = 0$ at $\omega = 0$

Quantum Brownian motion and the Third Law of thermodynamics

Peter Hänggi, Michele Campisi,
Gert-Ludwig Ingold, and Peter Talkner

Uni Augsburg

Acta Phys. Pol. B **37**, 1537 (2006)
New J. Phys. **10**, 115008 (2008)
Phys. Rev. E **79**, 061105 (2009)
J. Phys. A (Fast Track) **42**, 392002 (2009)

Model for a damped free particle

Hamiltonian

$$H = H_S + H_B + H_{SB}$$

$$= \frac{p^2}{2M} + \sum_{n=1}^{\infty}\left(\frac{p_n^2}{2m_n} + \frac{m_n}{2}\omega_n^2 x_n^2\right) + \sum_{n=1}^{\infty}\left(-c_n x_n q + \frac{c_n^2}{2m_n\omega_n^2}q^2\right)$$

translational invariance: $c_n = m_n\omega_n^2$

$$= \frac{p^2}{2M} + \sum_{n=1}^{\infty}\left(\frac{p_n^2}{2m_n} + \frac{m_n}{2}\omega_n^2 (x_n - q)^2\right)$$

Quantum Langevin equation

$$M\frac{\mathrm{d}^2}{\mathrm{d}t^2}q + M\int_{t_0}^{t}\mathrm{d}s\gamma(t-s)\frac{\mathrm{d}}{\mathrm{d}s}q = \xi(t)$$

damping kernel and noise

Drude model

damping kernel

$$\gamma(t) = \gamma\omega_{\mathrm{D}}\mathrm{e}^{-\omega_{\mathrm{D}}t}$$

Quantum Langevin equation

$$M\frac{\mathrm{d}^2}{\mathrm{d}t^2}q + M\gamma\omega_{\mathrm{D}}\int_{t_0}^{t}\mathrm{d}s\,\mathrm{e}^{-\omega_{\mathrm{D}}(t-s)}\frac{\mathrm{d}}{\mathrm{d}s}q = \xi(t)$$

equivalent equations of motion

$$\dot{q} = v$$

$$\dot{v} = z$$

$$\dot{z} = -\omega_{\mathrm{D}}z - \gamma\omega_{\mathrm{D}}v$$

oscillations occur for $\omega_{\mathrm{D}} < 4\gamma$

A bit of thermodynamics

$$\beta = \frac{1}{k_\mathrm{B} T}$$

$$\begin{tikzcd}[column sep=small]
 & \boxed{\text{density of states } \rho} & \\
 & \boxed{\text{canonical partition function } \mathcal{Z}} \arrow[u, "\mathcal{Z} = \int \mathrm{d}E \rho(E) \mathrm{e}^{-\beta E}"'] \arrow[dl, "U = -\frac{\partial \ln \mathcal{Z}}{\partial \beta}"'] \arrow[dr, "S = -\frac{\partial F}{\partial T} = -\frac{\partial k_\mathrm{B} T \ln \mathcal{Z}}{\partial T}"] & \\
\boxed{\text{internal energy } U} \arrow[dr, "C = \frac{\partial U}{\partial T}"'] & & \boxed{\text{entropy } S} \arrow[dl, "C = T \frac{\partial S}{\partial T}"] \\
 & \boxed{\text{specific heat } C} &
\end{tikzcd}$$

An important difference

Route I

$$E \doteq E_{\mathrm{S}} = \langle H_{\mathrm{S}} \rangle = \frac{\mathrm{Tr}_{\mathrm{S+B}}(H_{\mathrm{S}} \mathrm{e}^{-\beta H})}{\mathrm{Tr}_{\mathrm{S+B}}(\mathrm{e}^{-\beta H})}$$

Route II

$$\mathcal{Z} = \frac{\mathrm{Tr}_{\mathrm{S+B}}(\mathrm{e}^{-\beta H})}{\mathrm{Tr}_{\mathrm{B}}(\mathrm{e}^{-\beta H_{\mathrm{B}}})} \qquad U = -\frac{\partial \ln \mathcal{Z}}{\partial \beta}$$

$$\begin{aligned} \Rightarrow U &= \langle H \rangle - \langle H_{\mathrm{B}} \rangle_{\mathrm{B}} \\ &= E_{\mathrm{S}} + \Big[\langle H_{\mathrm{SB}} \rangle + \boxed{\langle H_{\mathrm{B}} \rangle - \langle H_{\mathrm{B}} \rangle_{\mathrm{B}}} \Big] \end{aligned}$$

For finite coupling E and U differ!

Thermodynamic argument:

$$\mathcal{Z} = \frac{\mathrm{Tr}_{\mathrm{S+B}}(\mathrm{e}^{-\beta H})}{\mathrm{Tr}_{\mathrm{B}}(\mathrm{e}^{-\beta H_{\mathrm{B}}})} \qquad \longrightarrow \qquad F_{\mathrm{S}} = F - F_{\mathrm{B}}^{0}$$

F total system free energy
F_{B} bare bath free energy

With this form of free energy the three laws of thermodynamics are fulfilled.

P. Hänggi, G.-L. Ingold, P. Talkner, New J. Phys. **10**, 115008 (2008)
G.-L. Ingold, P. Hänggi, P. Talkner, Phys. Rev. E **79**, 061105 (2009)

Partition function and internal energy

undamped case

$$Z_0 = \frac{L}{\hbar}\left(\frac{2\pi m}{\beta}\right)^{1/2}$$

with damping

$$Z = Z_0 \prod_{n=1}^{\infty} \frac{\nu_n}{\nu_n + \hat{\gamma}(\nu_n)}$$

internal energy compare with energy E

$$U = \frac{1}{2\beta}\left[1 + 2\sum_{n=1}^{\infty} \frac{\hat{\gamma}(\nu_n) - \nu_n \hat{\gamma}'(\nu_n)}{\nu_n + \hat{\gamma}(\nu_n)}\right]$$

$$= \frac{\hbar\omega_{\mathrm{D}}}{2\pi}\psi\left(\frac{\hbar\beta\omega_{\mathrm{D}}}{2\pi}\right) - \frac{x_+}{\beta}\psi(x_+) - \frac{x_-}{\beta}\psi(x_-) - \frac{1}{2\beta}$$

Specific heat from partition function

$$\frac{C^Z}{k_\mathrm{B}} = x_1^2\psi'(x_1) + x_2^2\psi'(x_2) - \left(\frac{\hbar\beta\omega_\mathrm{D}}{2\pi}\right)^2 \psi'\left(\frac{\hbar\beta\omega_\mathrm{D}}{2\pi}\right) - \frac{1}{2}$$

with

$$x_{1,2} = \frac{\hbar\beta\omega_\mathrm{D}}{4\pi}\left(1 \pm \sqrt{1 - \frac{4\gamma}{\omega_\mathrm{D}}}\right)$$

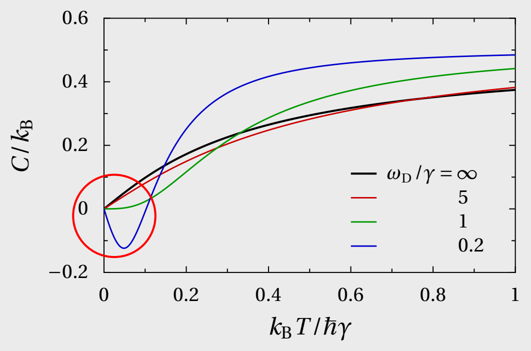
high-temperature expansion

$$\frac{C^Z}{k_\mathrm{B}} = \frac{1}{2} - \frac{\hbar^2\gamma\omega_\mathrm{D}}{12(k_\mathrm{B}T)^2} + \mathrm{O}(T^{-3})$$

low-temperature expansion

$$\frac{C^Z}{k_\mathrm{B}} = \frac{\pi}{3}\frac{k_\mathrm{B}T}{\hbar\gamma}\left(1 - \frac{\gamma}{\omega_\mathrm{D}}\right) - \frac{4\pi^3}{15}\left(\frac{k_\mathrm{B}T}{\hbar\gamma}\right)^3\left[1 - 3\frac{\gamma}{\omega_\mathrm{D}} - \left(\frac{\gamma}{\omega_\mathrm{D}}\right)^3\right] + \mathrm{O}(T^5)$$

return

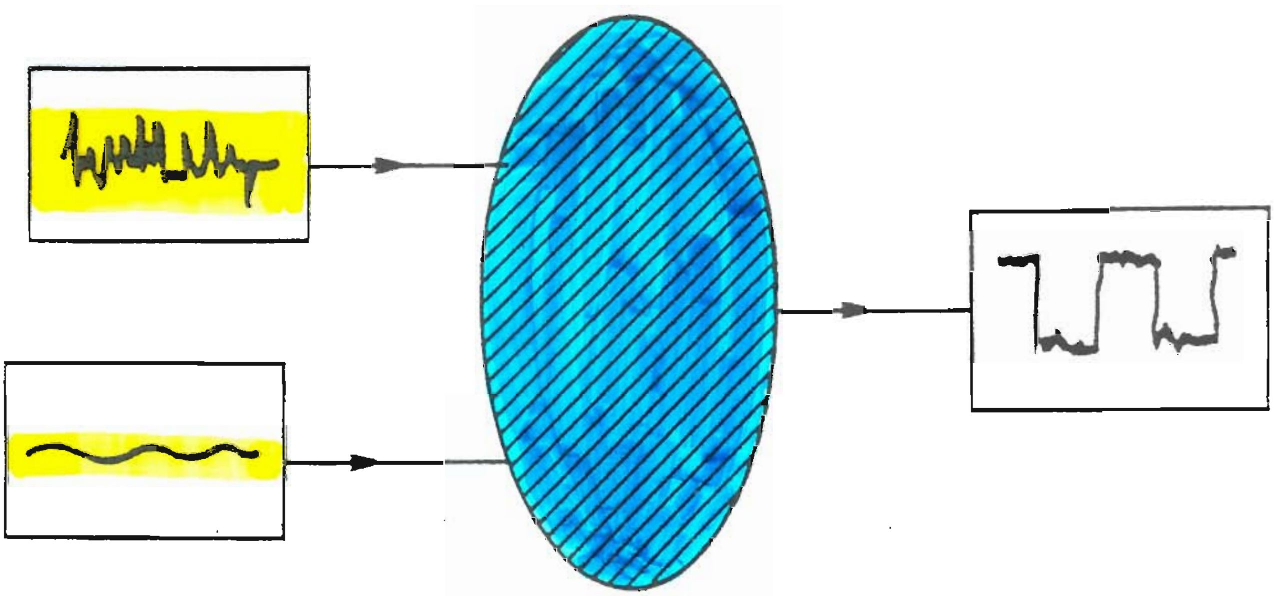


P. Hänggi, GLI, P. Talkner, New J. Phys. **10**, 115008 (2008)

damping kernel: $\gamma(t) = \gamma\omega_D e^{-\omega_D t}$

$$\hat{\gamma}(z) = \frac{\gamma\omega_D}{z+\omega_D}$$

SR



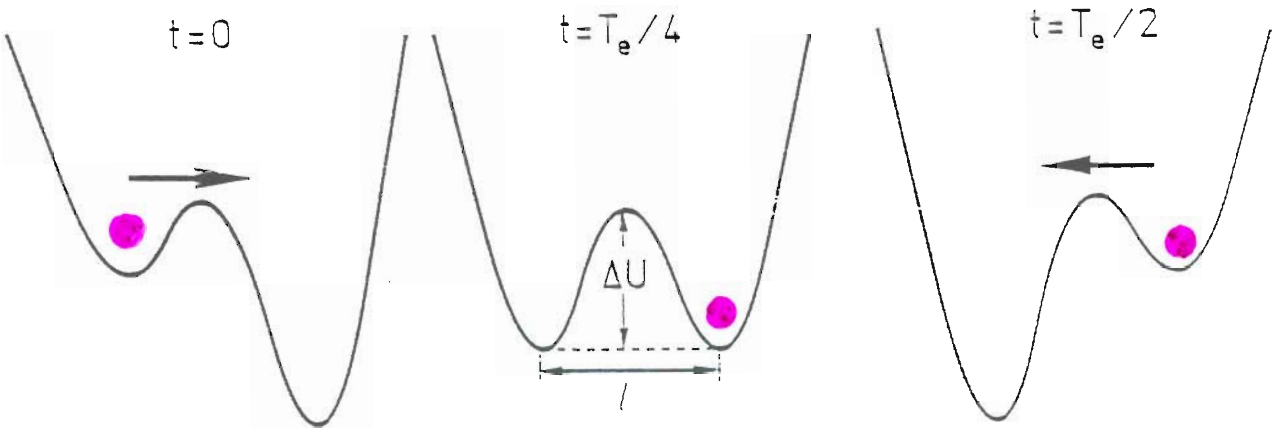
Schematic of stochastic resonance . The cross-hatched oval represents a black-box system which receives two inputs: one weak and periodic, the other strong and random. The output is relatively regular with small fluctuations.

Bistable Model

$$\dot{x} = x - x^3 + A\cos(\Omega t + \varphi) + \xi(t)$$

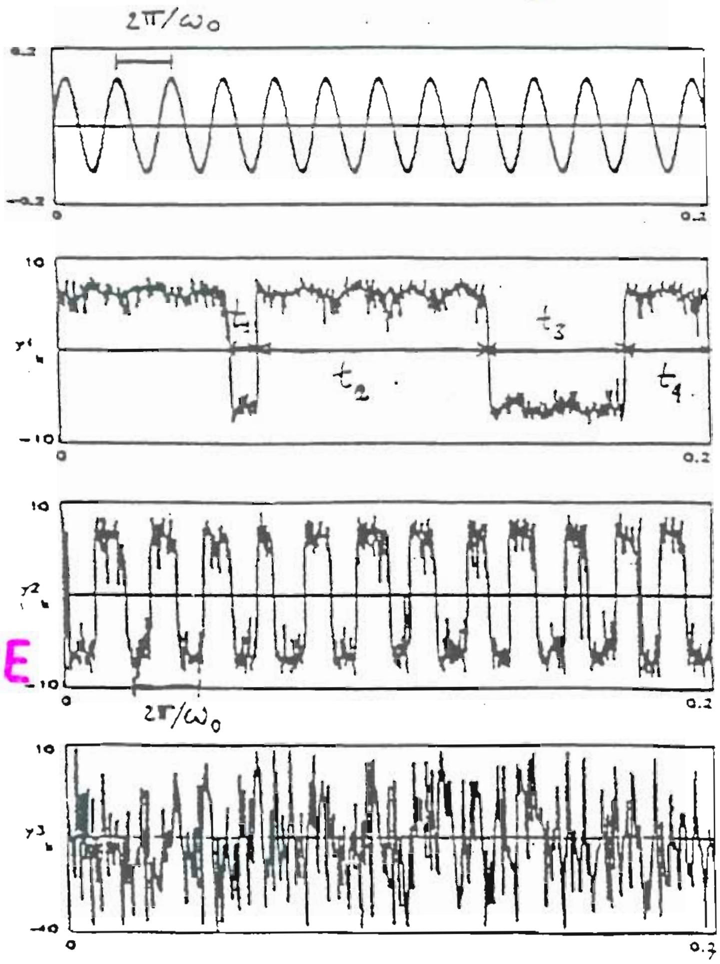
$$\langle \xi(t) \rangle = 0$$

$$\langle \xi(t)\xi(t') \rangle = 2D\,\delta(t - t')$$



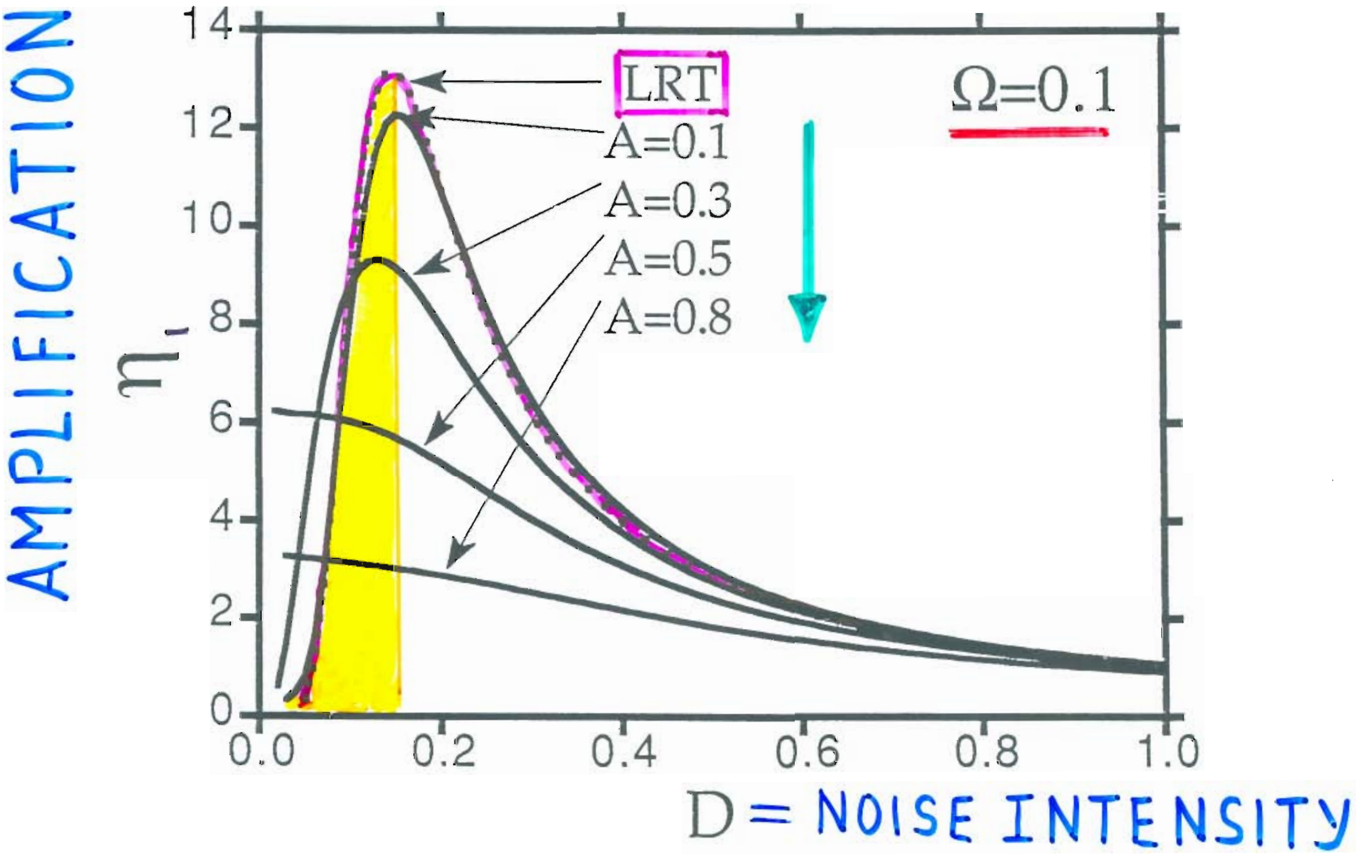
$$T_e = 2\pi / \Omega$$

SIGNAL



$$T_e \sim 2\Gamma^{-1}_{\text{ESCAPE}}$$

P. JUNG + P. H., PHYS. REV. A44: 8032 (91)



MORE NOISE → MORE SIGNAL

$$M_1 \sim \chi(\tau) = -\frac{1}{D}\frac{d}{d\tau}\langle \delta x(\tau)\,\delta\xi(0)\rangle$$

$$|M_1|^2 \propto \frac{1}{D^2} \qquad \exp(-2\Delta U/D)$$

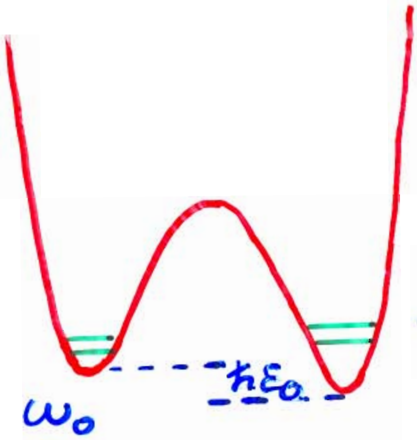
S R

IN QUANTUM MECHANICS

Q S R

$V_0 \gg \hbar\omega_0 \gg \hbar\varepsilon_0, kT$

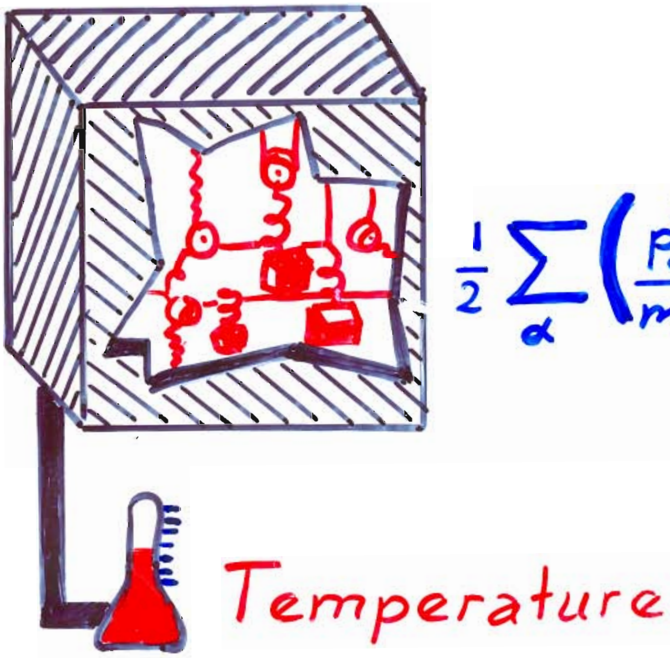
TS



$$-\frac{\hbar}{2}\left(\varepsilon_0\sigma_z + \Delta\sigma_x\right)$$

$\oplus$

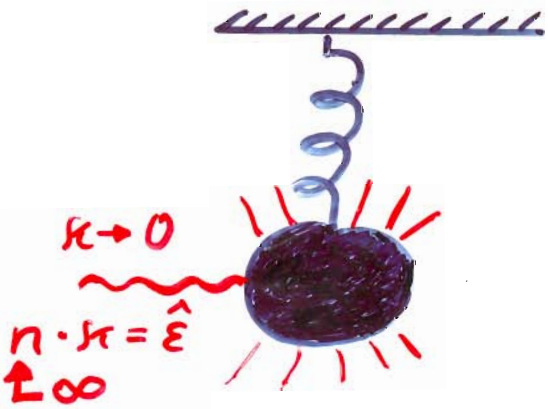
BATH
T, γ



$$\frac{1}{2}\sum_\alpha\left(\frac{p_\alpha^2}{m_\alpha} + m_\alpha\omega_\alpha^2 x_\alpha^2 - c_\alpha x_\alpha \sigma_z\right)$$

$\oplus$

DRIVE
$\Omega, \hat{\varepsilon}$



$$\frac{\hbar\hat{\varepsilon}}{2}\cos(\Omega t)\,\sigma_z$$

LINEAR RESPONSE & QSR

with $P_1 = \frac{A}{2} \chi_{qq}(\Omega) \equiv \frac{A}{2} \chi(\Omega)$

$$\eta_1 = 4\pi |P_1|^2 = \pi A^2 |\chi(\Omega)|^2$$

$$SNR = \frac{\pi A^2 |\chi(\Omega)|^2}{S_{qq}(\Omega, A=0)} = \frac{\pi A^2 |\chi(\Omega)|^2}{Im\, \chi(\Omega) \hbar \coth(\hbar\Omega\beta/2)}$$

¡valid at all temperatures!

PROBLEM: QUANTUM $\chi_{qq}(\Omega) \overset{FDT}{\rightsquigarrow} S_{qq}(\Omega)$

$$S_{qq}(t) = \frac{1}{2} \langle \delta\hat{q}(t)\delta\hat{q}(0) + \delta\hat{q}(0)\delta\hat{q}(t) \rangle_\beta$$

¡DIFFICULT!

LINEAR RESPONSE & QSR

with $P_1 = \frac{A}{2}\chi_{qq}(\Omega) \equiv \frac{A}{2}\chi(\Omega)$

$$\eta_1 = 4\pi |P_1|^2 = \pi A^2 |\chi(\Omega)|^2$$

$$\mathrm{SNR} = \frac{\pi A^2 |\chi(\Omega)|^2}{S_{qq}(\Omega; A=0)} = \frac{\pi A^2 |\chi(\Omega)|^2}{\mathrm{Im}\,\chi(\Omega)\,\hbar \coth(\hbar\Omega\beta/2)}$$

¡valid at all temperatures!

PROBLEM: QUANTUM $\chi_{qq}(\Omega) \overset{FDT}{\leftrightarrow} S_{qq}(\Omega)$

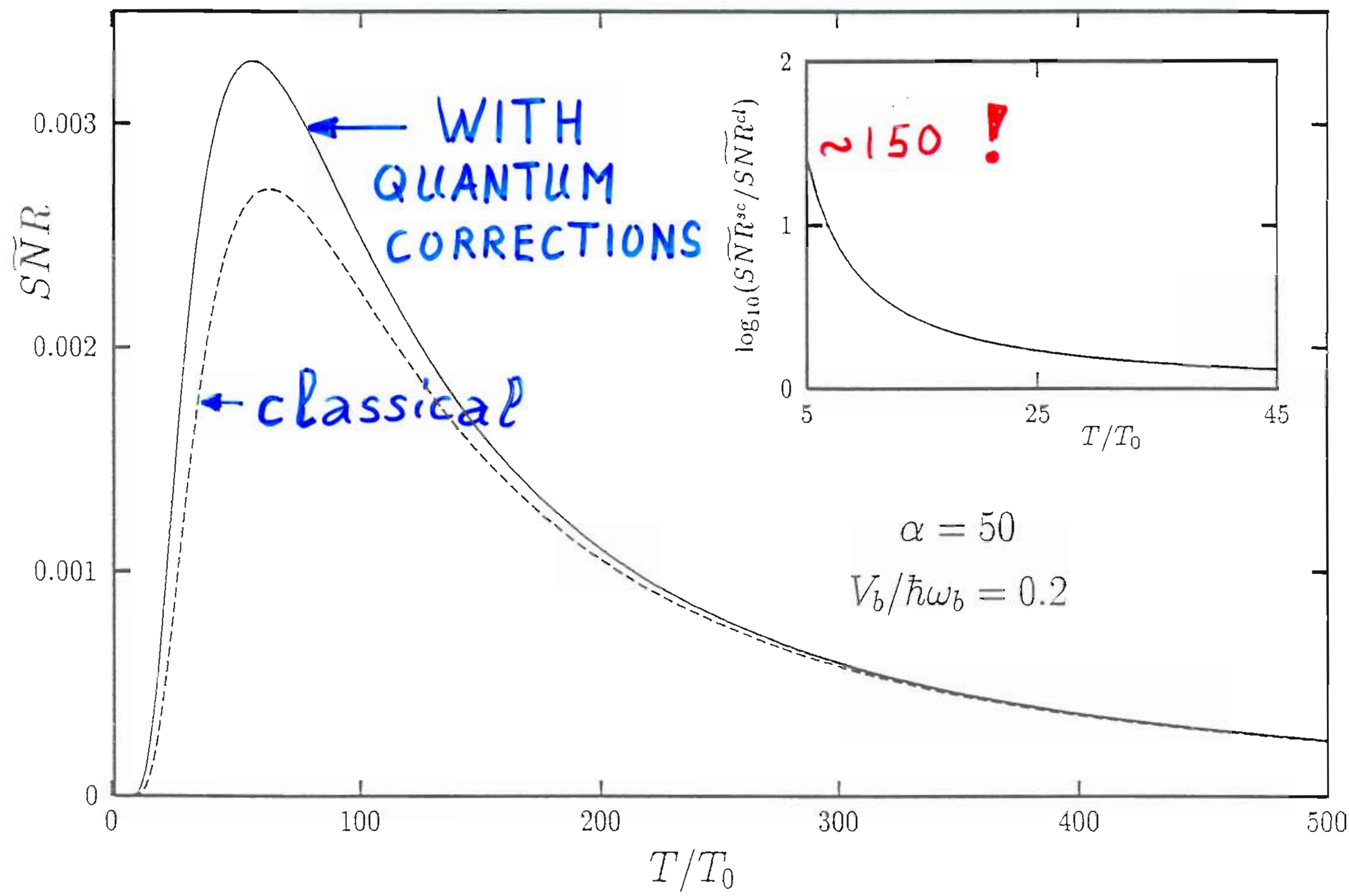
$$S_{qq}(t) = \frac{1}{2}\langle \delta\hat{q}(t)\delta\hat{q}(0) + \delta\hat{q}(0)\delta\hat{q}(t)\rangle_\beta$$

¡DIFFICULT!

2 LIMITS

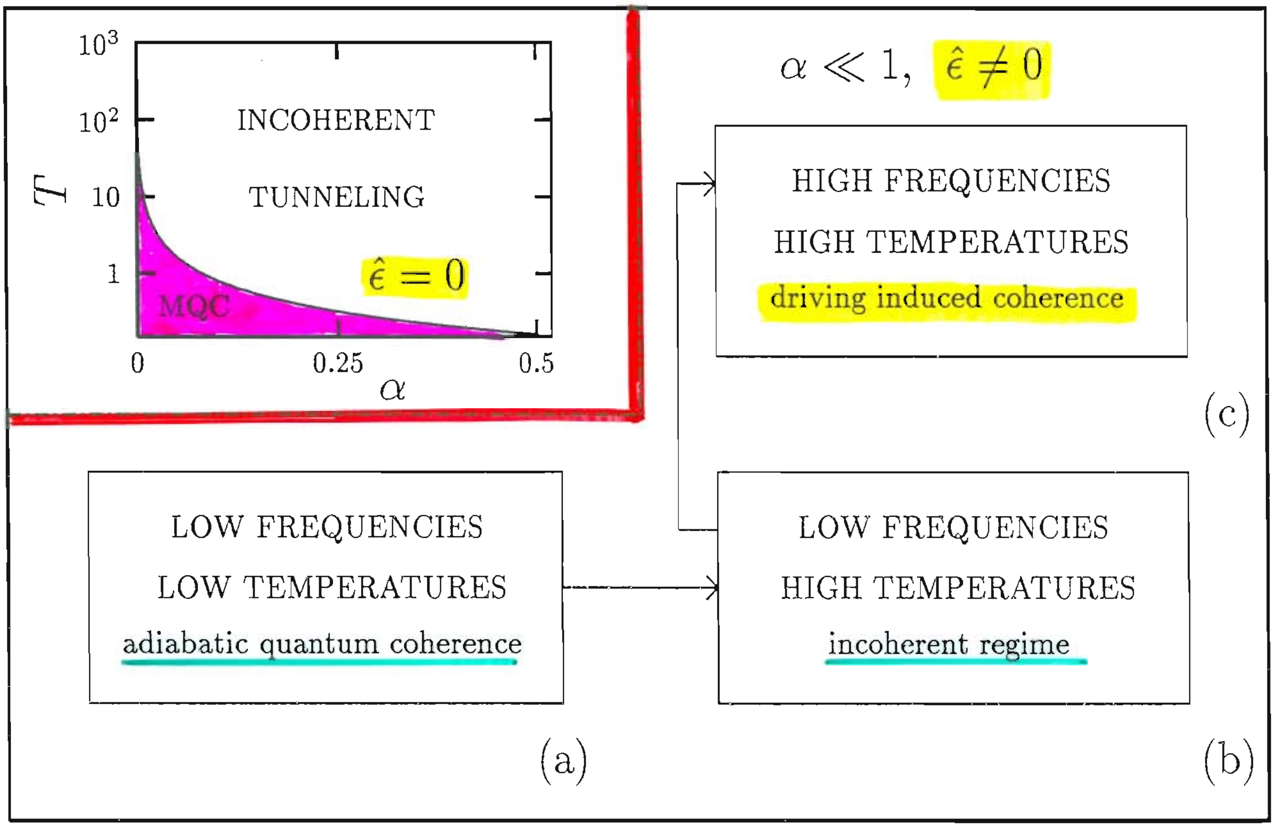
above ~ near crossover to thermal hopping

AT LOW T



0.003
0.002
0.001
0
0
100
200
300
400
500
$\widetilde{SNR}$
T/T_0
WITH QUANTUM CORRECTIONS
classical
$\alpha = 50$
$V_b/\hbar\omega_b = 0.2$
2
1
0
5
25
45
$\log_{10}(\widetilde{SNR}^{sc}/\widetilde{SNR}^{cl})$
T/T_0
~150 !

QUANTUM SR



10^3
10^2
10
1
T
INCOHERENT
TUNNELING
$\hat{\epsilon} = 0$
MQC
0
0.25
0.5
α
$\alpha \ll 1, \ \hat{\epsilon} \neq 0$
HIGH FREQUENCIES
HIGH TEMPERATURES
driving induced coherence
(c)
LOW FREQUENCIES
LOW TEMPERATURES
adiabatic quantum coherence
(a)
LOW FREQUENCIES
HIGH TEMPERATURES
incoherent regime
(b)

ENDE

FIN

THAT'S IT

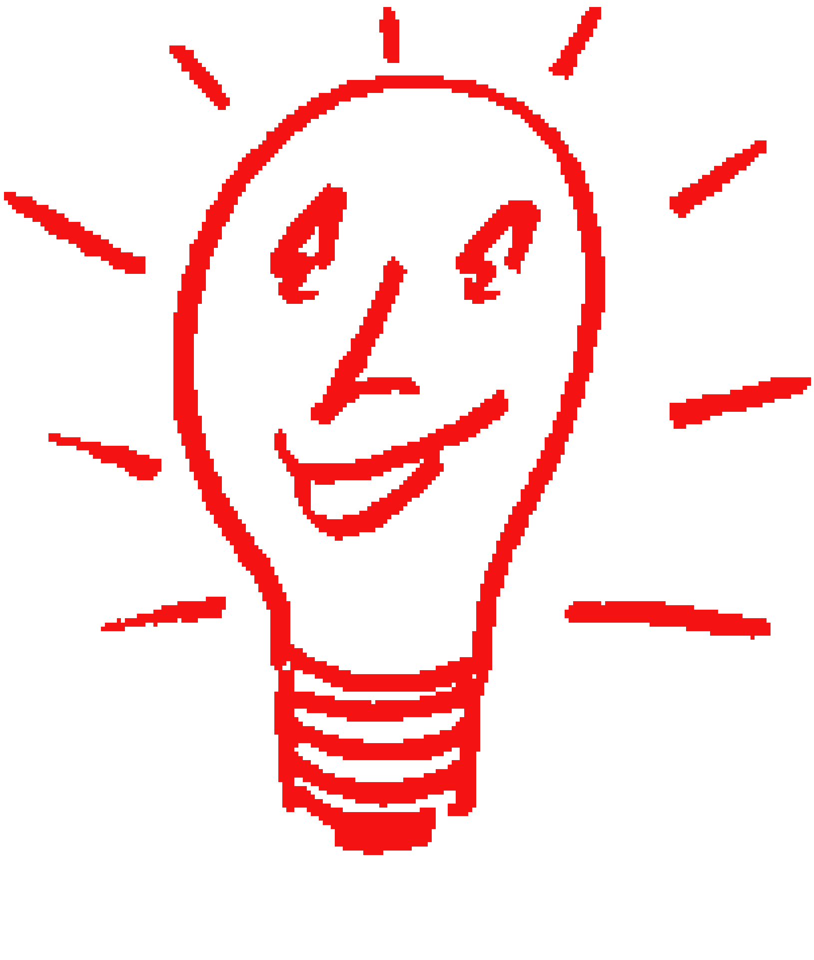
HOMEPAGE
„HANGGI“

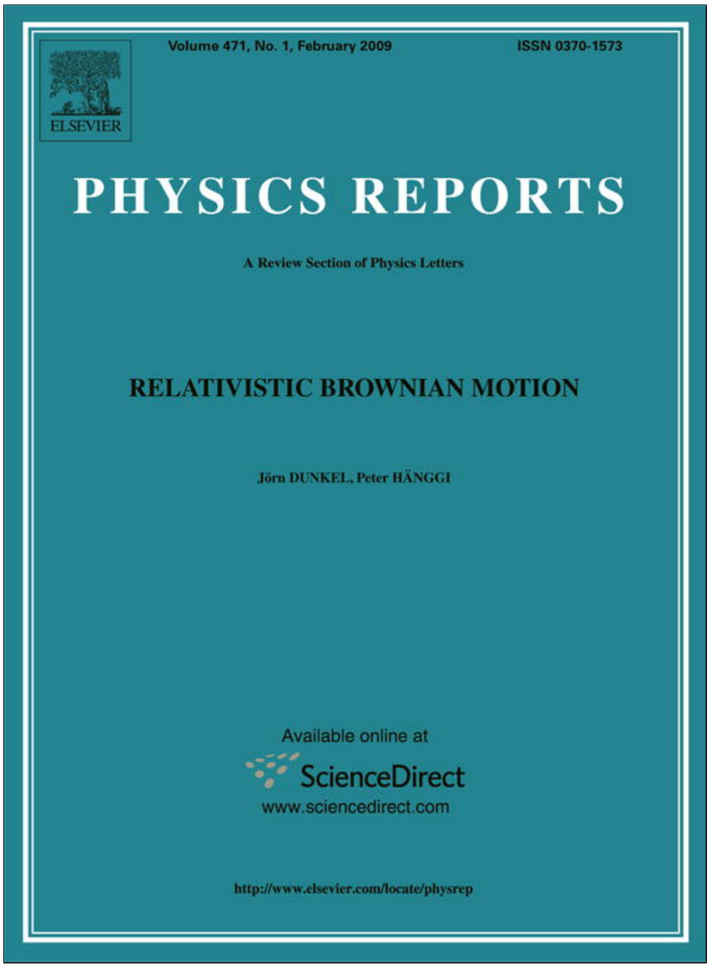
GO TO : FEATURE ARTICLES

- **Quantum Dissipation**
  and
  Quantum Transport

http://www.physik.uni-augsburg.de/theo1/hanggi/Quantum.html

A QUESTION ?




Volume 471, No. 1, February 2009
ISSN 0370-1573
ELSEVIER
PHYSICS REPORTS
A Review Section of Physics Letters
RELATIVISTIC BROWNIAN MOTION
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304: 229–358 (98)

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PHYSICS REPORTS (Review Section of Physics Letters) 168, No. 3 (1988) 115–207. North-Holland, Amsterdam

QUANTUM BROWNIAN MOTION: THE FUNCTIONAL INTEGRAL APPROACH

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Received January 1988

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Specific heat from the partition function

Route II

density of states ρ

canonical partition function $\mathcal{Z} = \dfrac{\mathrm{Tr}_{\mathrm{S+B}}\,(\mathrm{e}^{-\beta H})}{\mathrm{Tr}_{\mathrm{B}}\,(\mathrm{e}^{-\beta H_{\mathrm{B}}})}$

internal energy U

entropy S

specific heat C^{Z}

where β is the coefficient of sliding friction if there is slip between the diffusing molecule and the solution. For N molecules of solute per c.c. of solution the total resistance will be N times this, and in the steady state of diffusion will equilibrate the driving force due to variation of the osmotic pressure of the solute, namely dp/dx, which by the osmotic laws is $\mathrm{RT}\,dc/dx$, if c is the concentration of the solute at x and R is the gas constant. Hence

$dc = dN/C$

$$\mathrm{RT}\frac{dc}{dx} = 6\pi \mathrm{V}\eta a \mathrm{N}\frac{1+2\eta/\beta a}{1+3\eta/\beta a}\,; \quad . \quad . \quad . \quad . \qquad (2)$$

$NV = D\frac{dN}{dx} = \ldots$

and the required formula for the coefficient of diffusion with C for the number of molecules in a gramme-molecule is

$$\mathrm{D} = \frac{\mathrm{RT}}{6\pi\eta a \mathrm{C}}\,\frac{1+3\eta/\beta a}{1+2\eta/\beta a} \quad . \quad . \quad . \quad . \qquad (3)$$

If $\beta=\infty$, that is, if there is no slipping of solution at surface of molecule, $a\mathrm{D}$ is the same for all molecules diffusing through a given solvent at a given temperature. Now for a large molecule of solute moving amongst smaller ones of solvent, we can see that the slipping is probably small. But in the other extreme case of a small molecule of solute moving amongst larger ones of solvent, an effect analogous to slipping will occur, since the small molecule will travel a good deal in the gaps which would be left if the molecules of solvent were forced almost into permanent contact. We have thus two extreme cases of the formula.

$$\left.\begin{aligned} &\text{When } \beta=0, && \mathrm{D} = \frac{\mathrm{RT}}{4\pi\eta a\mathrm{C}} \\ &\text{and when } \beta=\infty, && \mathrm{D} = \frac{\mathrm{RT}}{6\pi\eta a\mathrm{C}} \end{aligned}\right\} \quad . \quad . \quad . \quad . \quad . \quad . \quad . \qquad (4)$$

Thus with increasing values of a we should have $a\mathrm{D}$ diminishing from the upper limit $\mathrm{RT}/4\pi\eta\mathrm{C}$, when a is small, to the lower limit $\mathrm{RT}/6\pi\eta\mathrm{C}$, when a is large. This is analogous to the actual behaviour of $\mathrm{B}^{\frac{1}{3}}\mathrm{D}$ obtained from experiment, B being the volume of the molecules in a gramme-molecule of solute. The first of the following tables contains the coefficients of diffusion for various gases through water determined by Hüfner *. I have reduced these all to a temperature of 16° C., and expressed them with the second as unit of time instead of the day. The values of B are taken mostly from "Further Studies on Molecular Force" (Phil. Mag. [6] xxxix.). In the second last row are given the values of

* Wied. *Ann.* 1897, vol. xl., and *Zeit. f. Phys. Chem.* xxvii.

QUANTUM NOISE

SYNOPSIS

LINEAR RESPONSE THEORY & QUANTUM-FDT

$$\hat{H}(t) = \hat{H}_0 - \mathcal{F}(t)\hat{A} \; ; \; \varrho_\beta = Z^{-1} \exp(-\beta \hat{H}_0)$$

$$\langle \hat{B}(t) \rangle - \langle \hat{B}(t) \rangle_\beta = \langle \delta \hat{B}(t) \rangle = \int_{t_0}^{t} \chi_{BA}(t-s)\, \mathcal{F}(s)\, ds$$

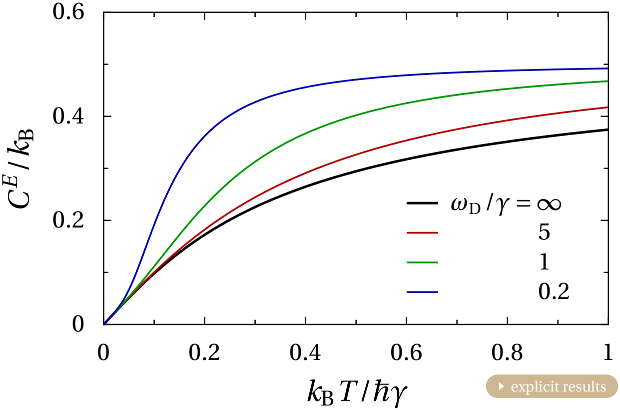
KUBO: $$\chi_{BA}(\tau) = \Theta(\tau) \frac{i}{\hbar} \langle [\hat{B}(\tau), \hat{A}(0)] \rangle_\beta$$

$$= -\Theta(\tau) \int_0^\beta \langle \hat{A}(-i\hbar\lambda) \dot{\hat{B}}(\tau) \rangle_\beta \, d\lambda$$

classical limit $\longrightarrow -\Theta(\tau)\, \beta \langle \dot{B}(\tau) A(0) \rangle_\beta$

Specific heat of a damped free particle

Route I

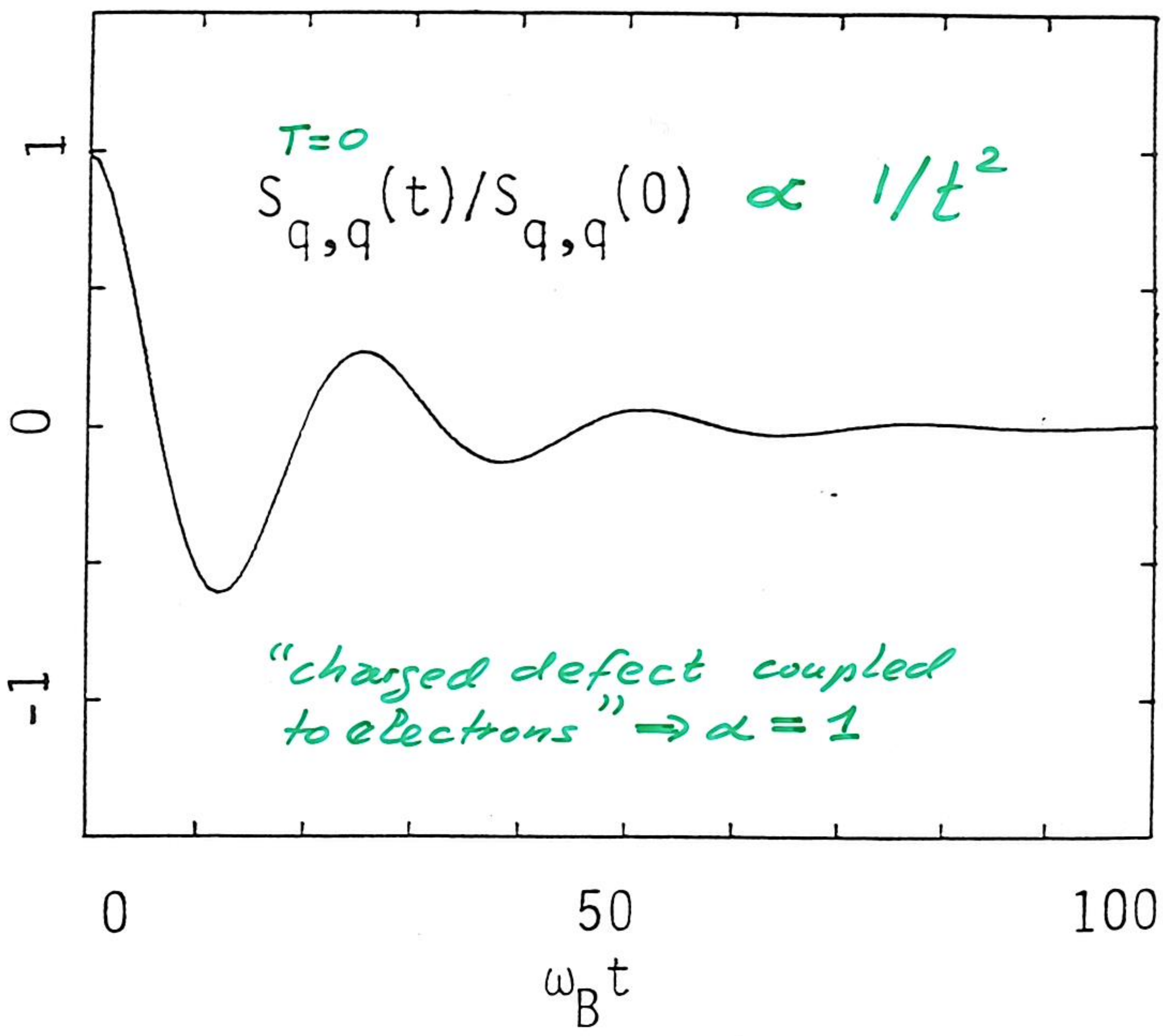


▸ explicit results

- $T \to \infty$: classical value $k_B/2$
  damping constant γ sets the temperature scale
- coupling to the environment ensures 3rd law
- less damping makes the system more classical

$U(q) = \frac{M_0}{2} \omega_0^2 q^2$, Ohmic friction $-\gamma \dot{q}-$

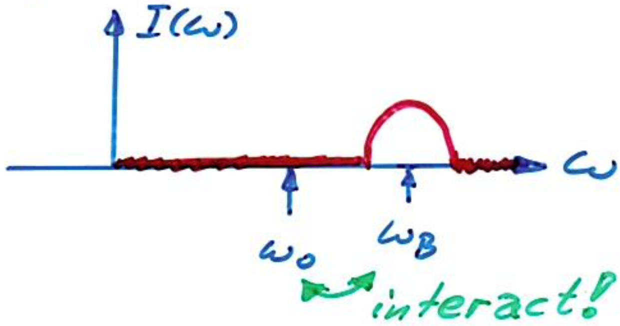
damped quantum harmonic oscillator

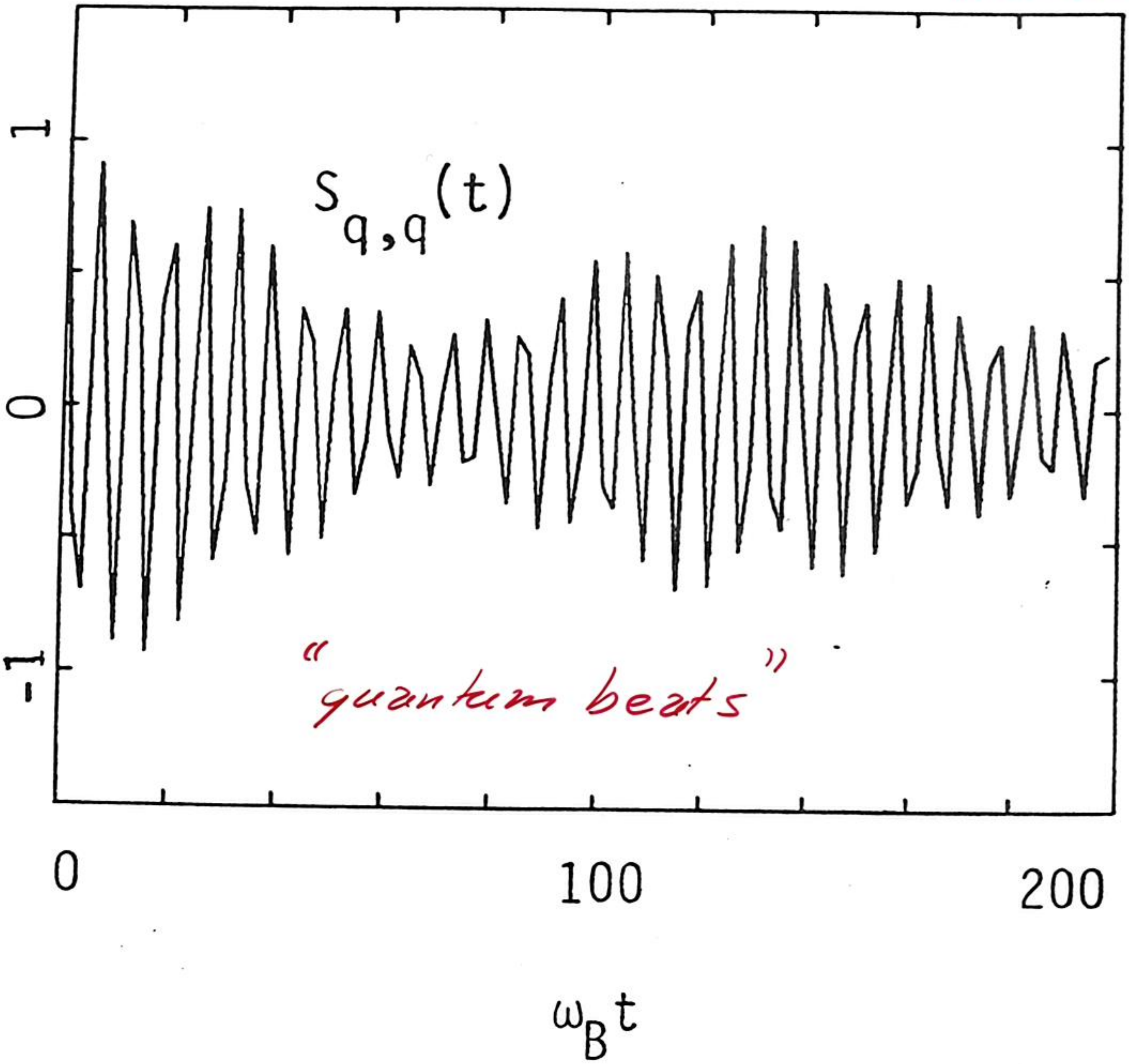


Riseborough, P.H., U. Weiss, Phys. Rev. **A31**, 471 (85)

$$U(q) = \frac{1}{2} M_0 \omega_0^{2} q^{2}$$

non-Ohmic friction





$$\hat{\gamma}(z) = \int_0^\infty \exp(-zt)\,\gamma(t)\,dt$$

$$\tilde{\gamma}(\omega) = \hat{\gamma}(z = -i\omega)$$

OHMIC DISSIPATION

$$J(\omega) = \gamma\,\omega \exp(-\omega/\omega_c)$$

cut-off frequency

$\omega_c \gg \omega_0, \omega_b$

KONDO-PARAMETER

$$= \underbrace{(2\pi\hbar/a^2)\,\boxed{\alpha}}_{=\gamma}\,\omega \exp(-\omega/\omega_c)$$

$a = 2q_a$: tunneling length