Quantum Dissipation: A Primer

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QUANTUM DISSIPATION $\mathcal{L} = \frac{1}{2} m_0 e^{xt_2} - \frac{1}{2} m_0 e^{xt_2}^2$ L'éco

d dL = d moex = moex + moex



 $QM: L \rightarrow H = \frac{p^2}{2m_0}e^{-yt} + \frac{1}{2}m_0e^{st}\omega_0^2x^2$







NOISE-INDUCED ESCAPE



rate = $F(y) = \frac{\omega_0}{2\pi} \exp(-\delta U/D)$ RMP 62: 251(90)



thermal equilibrium P.H., P. TALKNER, M. BORKOVEC REV. MOD. PHYS. <u>62</u>: 251(1990)

Reaction-rate theory: fifty years after Kramers

Peter Hänggi, Peter Talkner, Michal Borkovec

RMP 62: 251 (90)

THE PROBLEM





FACTS

D







H2& HD sorbed in Zeolites [Bouchand etal (92)



CO-MIGRATION IN HEHOGLOBIN [Frauenfelder]



TUNNELING IN A JOSEPHSON JUNCTION SUBJECTED TO MEMORY FRICTION [Esteve et. al. (79)]

Results

Quantum Tunneling	Cross- over	Quantum Corrections	thermal T activation T
R=Aexp-B	2-0-mode	$k = F_{ep} Q$	$k = A(n)e^{-E_0/AT}$
$B=S_{B}(T,\gamma)$	$\frac{S_B}{E} = \frac{E_b}{E}$	quantum enhancement	y=n/M
B(T=0)= B(T=0) -a T ² !	smooth!	$Q \sim exp \frac{\hbar^2(\omega_o^2 + \omega_o^2)}{(kT)^2}$	$\left\{\left(\frac{3}{4}+c_{0}^{2}\right)^{2}-\frac{3}{2}\right\}$
$A(T_{i}y) \simeq A(y)$ $\exists l_2$	Erfc- behavior	>1 i.e.	· 600
« A (1+2.80x), y→0 2.400		$E_b \rightarrow E_b - \frac{c}{T}$	

Quantum transmission coefficient



- red Redfield
- black path integral
- blue quantum Grote-Hynes theory
- brown quantum turnover theory by Hänggi, Pollak, Grabert
- green quantum turnover theory by Rips and Pollak
- triangles centroid method

Reaction-rate theory: fifty years after Kramers

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The calculation of rate coefficients is a discipline of nonlinear science of importance to much of physics, chemistry, engineering, and biology. Fifty years after Kramers' seminal paper on thermally activated barrier crossing, the authors report, extend, and interpret much of our current understanding relating to theories of noise-activated escape, for which many of the notable contributions are originating from the communities both of physics and of physical chemistry. Theoretical as well as numerical approaches are discussed for single- and many-dimensional metastable systems (including fields) in gases and condensed phases. The role of many-dimensional transition-state theory is contrasted with Kramers' reaction-rate theory for moderate-to-strong friction; the authors emphasize the physical situation and the close connection between unimolecular rate theory and Kramers' work for weakly damped systems. The rate theory accounting for memory friction is presented, together with a unifying theoretical approach which covers the whole regime of weak-to-moderate-to-strong friction on the same basis (turnover theory). The peculiarities of noise-activated escape in a variety of physically different metastable potential configurations is elucidated in terms of the mean-first-passage-time technique. Moreover, the role and the complexity of escape in driven systems exhibiting possibly multiple, metastable stationary nonequilibrium states is identified. At lower temperatures, quantum tunneling effects start to dominate the rate mechanism. The early quantum approaches as well as the latest quantum versions of Kramers' theory are discussed, thereby providing a description of dissipative escape events at all temperatures. In addition, an attempt is made to discuss prominent experimental work as it relates to Kramers' reaction-rate theory and to indicate the most important areas for future research in theory and experiment.

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				\boldsymbol{q}_i	configurational degree of freedom
A (7	7)	temperature-dependent quantum rate pr	efac-	r(E)	quantum reflection coefficient
		tor		s(x)	density of sources and sinks
C(t)		correlation function		t(E)	quantum transmission coefficient
D		diffusion coefficient		$t_{\Omega}(x)$	mean first-passage time to leave the domain
Ε		energy function			Ω , with the starting point at x
\overline{E} .		activation energy $(=$ harrier energy with	the	<i>t</i> MEDT	constant part of the mean first-passage time
™ b		energy at the metastable state set equal	to	· MFP1	to leave a metastable domain of attraction
		zero)		$v = \dot{r}$	velocity of the reaction coordinate
$\mathbf{F}^{(A)}$		Lowin matrix of the anarry function	. +	r	reaction coordinate
Ľ		the stable state	ai	л Т. Т	location of well minimum or notantial
$\mathbf{F}^{(S)}$		Hessian matrix of the energy function		$\boldsymbol{x}_0, \boldsymbol{x}_a$	minimum of state 4 manualius
12		around the saddle-point configuration		r .	harrier location
		around the saddle-point configuration		harmondless b	Ualiter invation

 x_T β location of the transition state inversion temperature $(k_B T)^{-1}$

action variable of the reaction coordinate

J Jacobian

Ι

microscopic approach

 $H^{+otal} = \frac{1}{2}M\dot{q}^{2} + ll(q)$ system

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

+ q Z Ca ga linear coupling $+q^2\sum_{\alpha}\frac{c_{\alpha}}{2m_{1}c_{1}^2}$

compensation of frequency shift

QE.

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



QUANTUM NOISE

QUANTUM L.-EQ.



$\frac{|0\rangle_{S+B}}{4} \neq \frac{|0\rangle_{S}}{2}$ $\frac{|0\rangle_{B}}{4}$ $\frac{|0\rangle_{S+B}}{4} \neq \frac{|0\rangle_{S}}{2}$ $\frac{|0\rangle_{S+B}}{4} \neq \frac{|0\rangle_{S}}{2}$

$H_{s+n} = H_s + H_{s-n} + H_B$

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

Ss #2" exp (- Hs)

 $S_{Total} = S_{s+B} = 2^{-1} e_{xp} \left(-\frac{H_{s+B}}{hT}\right)$

5 QLE $i_{x}\dot{o} = [O, H_{-}]$ $m\ddot{x} + m \int ds y(t-s) \dot{x}(s) + \frac{\partial V(x)}{\delta x}$ $= \eta(t) - m_{g}(t-0) \times (0)$ INITIAL SLIP $\gamma(t-s) = \frac{1}{m} \sum_{m,\omega^2} \frac{c_{\alpha}}{\cos(\omega_{\alpha}(t-s))}$ $= \gamma(s-t)$

 $m(t) = \sum_{n} \sum_{n} \left[q_n^{(0)} \cos(\alpha_n t) + \frac{\mu_n}{m_n \omega_n} \sin(\alpha_n t) \right]$





• $\frac{1}{2} < m(t) m(ss + m(ssm(t))) = C(t-s)$ $= C(\tau) = \frac{\pi}{2} \sum_{n} \frac{c_n}{c_n} \coth\left(\frac{\pi c_n}{2\Lambda T}\right) \cosh(\frac{\pi}{2\Lambda T})$

 $\hat{\mathbf{x}}(z) = \int e^{z} e^{-zt} dt$ $\delta(\omega) = \int (z = -i\omega)$ OHMIC DISSIPATION $J(\omega) = \chi \omega \exp(-\omega/\omega_e)$ cut-off frequency We >> Wo, Wh KONDO-PARAMETER, $= (2\pi \hbar / a^2) \propto \omega \exp(-\omega / \omega_c)$ a=29a: tunneling length

REMARKS

1.

QLE OPERATES IN FULL HILBERT SPACE OF SOB

 $\hat{g}(z) = \int e^{izt} g(t)dt = \frac{i}{2m} \sum_{\alpha} \frac{c_{\alpha}}{\alpha} \left[\frac{1}{z - c_{\alpha}} + \frac{1}{z + c_{\alpha}} \right]$ $\frac{1}{x+iot} = P(\frac{1}{x}) - i\pi S(x) \qquad \text{Im} \geq 0$ $Re_{g}^{2}(2 = \omega + iot) = \frac{\pi}{2m} \sum_{\alpha} \frac{c_{\alpha}}{m_{\alpha}\omega_{\alpha}^{2}} \left[d(\omega - \omega_{\alpha}) + d(\omega + \omega_{\alpha}) \right]$ $- C(\tau) = \frac{m}{\pi} \int d\omega \operatorname{Re}_{\mathcal{S}} (\omega + i0^{\dagger}) \cos(\omega \tau)$ · coth (the) 3 with $\mathfrak{J}(t) = \mathfrak{l}(t) - \mathfrak{m}_{\mathfrak{f}}(t) \times (0)$ $\hat{S}_{B} = 2^{-\prime} e_{xp} - \beta \left[\sum_{\alpha} \left(\frac{p_{\alpha}^{2}}{2m_{\alpha}} + \frac{m_{\alpha}^{2} v_{\alpha}^{2}}{2} \left(q_{\alpha} - \frac{c_{\alpha}}{2m_{\alpha}} \right) \right]$ → < ğ(t)> = 0 $\frac{2}{2} < \frac{3}{7} + \frac{3}{7} + \frac{3}{7} + \frac{3}{7} = C(\tau)$



 $\langle \times (0) \} (t) \neq 0$

 $\langle H_{int} \rangle_{p} \neq 0$



SYNOPSIS LINEAR RESPONSE THEORY & QUANTUM-FDT

 $\hat{H}(t) = \hat{H}_{o} - F(t)\hat{A}; s_{\rho} = Z \exp(-\beta \hat{H}_{o})$ $\langle \hat{B}(t) \rangle - \langle \hat{B}(t) \rangle = \langle \delta \hat{B}(t) \rangle = \int \chi(t-s) \mathcal{F}(s) ds$ $K \sqcup BO: \chi_{BA}(\tau) = \Theta(\tau) \stackrel{i}{\leftarrow} \langle [\hat{B}(\tau), \hat{A}(o)] \rangle_{BA}$ $= -\Theta(\tau) \hat{S} \langle \hat{A}(-i \pm \lambda) \hat{B}(\tau) \rangle d\lambda$ classical limit - OUT) B< BIT) A10)>

SYNOPSIS LINEAR RESPONSE THEORY & QUANTUM-FDT

 $\hat{H}(t) = \hat{H}_{o} - F(t)\hat{A}; s_{\rho} = Z \exp(-\beta \hat{H}_{o})$ $\langle \hat{B}(t) \rangle - \langle \hat{B}(t) \rangle_{\beta} = \langle \delta \hat{B}(t) \rangle = \int \chi(t-s) \mathcal{F}(s) ds$ $KUBO: \chi_{BA}(\tau) = \Theta(\tau) \frac{i}{\tau} \langle [\hat{B}(\tau), \hat{A}(\omega)] \rangle_{BA}$ $= -\Theta(\tau) \hat{S} \langle \hat{A}(-i \pm \lambda) \hat{B}(\tau) \rangle d\lambda$ classical limit - OUT) B< BIT) A10)> $\hat{B} = \hat{A} = \hat{q}$; $\mathcal{F}(t) = A \cos \Omega t$ < Jq(+)> = P, e-ist + P, e-ist $P_{1-1} = \frac{A}{2} e^{\mp i \Omega t} \chi(\pm \Omega)$

QUANTUM-FDT

 $S_{BA}(\tau) = \frac{1}{2} < (\hat{B}(t) - \langle \hat{B} \rangle) (\hat{A}(0) - \langle \hat{A} \rangle)$ + $(\hat{A}(0) - \langle \hat{A} \rangle_{p}) (\hat{B}(\tau) - \langle \hat{B} \rangle_{p})$ $\chi_{BA}(\tau) = \chi'_{BA}(\tau) + i \chi''_{BA}(\tau)$ $\frac{1}{2} \begin{bmatrix} \chi_{BA}(+) + \chi_{AB}(-t) \end{bmatrix} - \frac{1}{2} \begin{bmatrix} \chi_{BA}(+) - \chi_{AB}(-t) \end{bmatrix}$ $\chi_{BA}(\omega) = \int_{\omega} \chi_{BA}(t) e^{i\omega t} dt$ $\chi''_{BA}(\omega) = \frac{1}{\pi} \tanh(\pi\omega\rho/2) S_{BA}(\omega)$ $S_{BA}(\omega) = \hbar \coth(\hbar\omega \beta/2) \chi_{BA}'(\omega)$ 2 X BA(C) (BSU) NOTE: $\chi''_{BA}(\omega) = \frac{1}{2} \left[\chi^*_{AB}(\omega) - \chi_{BA}(\omega) \right]$ $\neq Im \chi_{BA}(\omega)$; except $\lambda = \hat{B}$ $\hat{A} = \hat{B} = \hat{q} : S_{qq}(\Omega) = \hbar \cosh(\hbar \Re \beta 2) \operatorname{Im} \chi_{qq}(\mathcal{Q})$



 $S_{II}(\omega) = (\hbar \omega) \cosh\left(\frac{\hbar \omega}{2\hbar T}\right) Re 2(\omega)$

kT>>ta: SII(w) -> 2kT Re 2(w) TARMY 21T/R

JOHNSON-NYQUIST (1928)

- tw Re Z(w) ht << tw quantum-zero point fluct. S. (w=0) = 0 at w=0

1900-1951

J.B. Johnson

Thermal agitation of electricity in conductors.

Phys. Rev. (1928) 32 (July) 97-109

H. Nyquist

Thermal agitation of electric charge in conductors.

Phys. Rev. (1928) 32 (July) 110-113

L. Onsager

Reciprocal relation in irreversible process.

Phys. Rev. (1931) 32 (February) 405-426

H.B. Callen, T.A. Welton

Irreversibility and Generalized Noise.

Phys. Rev. (1951) 83 (1) 34-40

QUANTUM NOISE



NO QUANTUM EQ. PARTITION-TH.



S:= 14, (+)>< 42(+) ; u:=== Sdw - 500

 $i \hbar \hat{g} = [H_{0,g}] + \underbrace{\#} [\chi^{2}_{g}] - \underbrace{$(+)[\chi,g]} - \underbrace{\#} [\chi^{2}_{g}] - \underbrace{[\chi^{2}_{g}] - \underbrace{[\chi^{2}_{g}]} - \underbrace{[\chi^{2}_{g}]} - \underbrace{[\chi^{2}_{g}] - \underbrace{[\chi^{2}_{g}]} - \underbrace{[\chi^{2}_{g}]} - \underbrace{[\chi^{2}_{g}] - \underbrace{[\chi^{2}_{g}]} - \underbrace{[\chi^{2}_{g}]} - \underbrace{[\chi^{2}_{g}]} - \underbrace{[\chi^{2}_{g}] - \underbrace{[\chi^{2}_{g}]} - \underbrace{[\chi^{2}_{g}]} - \underbrace{[\chi^{2}_{g}] - \underbrace{[\chi^{2}_{g}]} - \underbrace$

PIT FALLS

MARKOV MASTER EQ

 $\frac{d}{ds} = -\frac{1}{2}Ls - \Gamma_s + I(t)$

BLOCH-REDFIELD i.g. NO DET. BALANCE ROTATING WAVE APPROX.

(LINDBLAD; DAVIES-APPROX.)

- DET. BALANCE V O.K. BUT
- WRONG EHRENFEST EQ.
- NO FDT
- NO KMS-COND. < u(t) = < u(t + in p)



Schematic of stochastic resonance. The crosshatched 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.



NOISE - ASSISTED SYNCHRONIZED HOPPING

Bistable Model



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



MORE NOISE -> MORE SIGNAL

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



MORE NOISE -> MORE SIGNAL

S R

IN QUANTUM MECHANICS

QSR



LINEAR RESPONSE 2QSR

with
$$P_1 = \frac{A}{2} \chi_{gg}(\mathcal{R}) \equiv \frac{A}{2} \chi(\mathcal{R})$$

$$\gamma_1 = 4\pi |P_1|^2 = \pi A^2 |\chi(\Omega)|^2$$

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

PROBLEM: QUANTUM X(S) S(S)

 $S_{gg}(t) = \frac{1}{2} < J_{q}(t) J_{q}(0) + J_{q}(0) J_{q}(t) >_{A}$ DIFFICULT

LINEAR RESPONSE 2QSR

with
$$P_1 = \frac{A}{2} \chi_{gg}(\mathcal{R}) \equiv \frac{A}{2} \chi(\mathcal{R})$$

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

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

PROBLEM: QUANTUM X(I) S(I)

 $S_{qq}(t) = \frac{1}{2} < \delta \hat{q}(t) \delta \hat{q}(0) + \delta \hat{q}(0) \delta \hat{q}(t) >_{\beta}$

DIFFICULT



above-near crossover to thermal hopping AT LOW T





=0; $M \frac{d^2}{d\tau^2} q_B(\tau) = \frac{\partial U}{\partial q_B}$ $- M \frac{d^2}{d\tau^2} \dot{q}_{B}(\tau) + \left(\frac{\partial^2 N}{\partial q^2}\right) \dot{q}_{B}(\tau) = 0$



. . .



 $\Theta = \hbar/kT$

$$q_{B}(\tau + \Theta) = q_{B}(\tau)$$

QUANTUM SR



DRIVEN QUANTUM TUNNELING

M. GRIFONI, P.H. PHYS. REP. <u>304</u>: 229–358(98)

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- BATH SPECTRUM
- . NOISE INPUT

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