QUANTUM DISSIPATION:

WHAT CAN AND CAN'T BE DONE

WITH OSCILLATOR BATHS

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Quantum System(S) Interacting with General Environment (E)

(Note: by definition of "E", we are not interested in it in its own right but only for its effects on S)

General prescription:

$$\hat{H} \equiv \hat{H}_s + \hat{H}_e + \hat{H}_{se} \quad . \qquad \Psi \equiv \Psi(\underset{S}{q}, \underset{E}{\{\xi\}})$$

eliminate environmental and coords $\{\xi\}$ to find effective description of S.

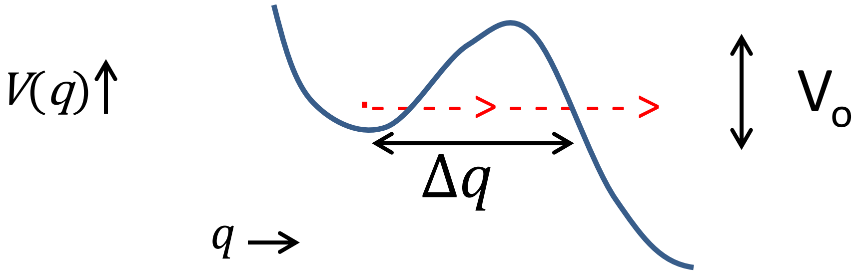
Feynman & Vernon (1963): for linearly dissipative system, model E by bath of simple harmonic oscillators with coupling linear in both oscillator and system coordinates, i.e.

$$\hat{H}_e = \sum_\alpha \left(p_\alpha^2/2m_\alpha + \frac{1}{2} m_\alpha {\omega_\alpha}^2 x_\alpha^2 \right) - \underset{\text{counter term}}{\underset{\uparrow}{(\text{C.T.})}}$$

$$\hat{H}_{SE} = -q \sum_\alpha C_\alpha x_\alpha^2$$

Note: linear response of SHO identical in classical + quantum mechanics! ⟶ can integrate out oscillators exactly.

AO Caldeira and AJL (1981): Apply FV technique to problem of quantum tunnelling of macroscopic variable (e.g. phase of Josephson junction) out of metastable well



"ohmic" dissipation

problem: how is escape rate affected by term $-\eta\dot{q}$ in classical equation of motion?

Friction coeff

To discuss this need to relate C_α's in FV description to η:

$$\sum_\alpha (|C_\alpha|^2 / m_\alpha \omega_\alpha) \delta\ (\omega - \omega_\alpha) \equiv J(\omega) = \eta\omega$$

Then find:

independent of η

$$\Gamma_{c\ell} = \omega_{c\ell}(\eta) \exp - V_O / k_B T \qquad \text{[Kramers, 1941]}$$

depends on η

$$\Gamma_{QM} = \omega_{QM}(\eta) \exp - S(\eta)/\hbar$$

WKB

depends on η

$$S(\eta) = S_O + \Delta S(\eta)$$

$$\Delta S(\eta) \sim \eta \iint dt dt' \left(\frac{q(\tau) - q(T')}{\tau - \tau'}\right)^2$$

$q(\tau)$ = "instanton" trajectory

thus to order of magnitude

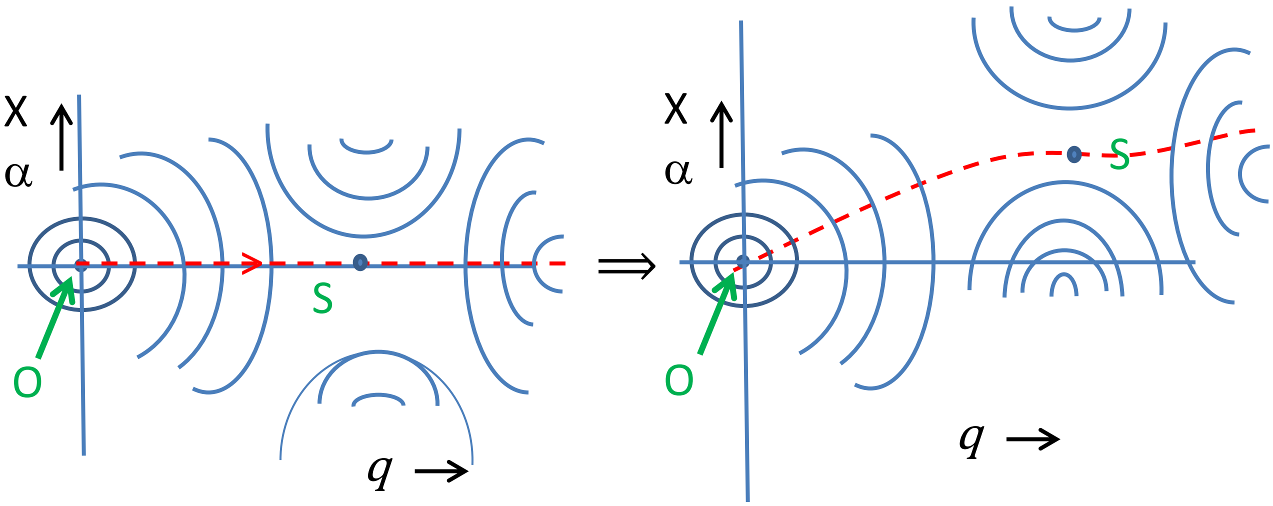
$$\Delta S(\eta) \sim \eta (\Delta q)^{2} / \hbar$$

ohmic dissipation always tends to suppress quantum Tunneling.

Question : Why does dissipation affect only prefactor in thermal activation, but exponent in quantum tunnelling?

Why does ohmic dissipation ($F_{fr} \propto \dot{q}$) affect only the prefactor of the Gibbs – Arrhenius (thermal) formula but the exponent of the WKB (quantum) formula?

Activation/tunnelling in many-dimensional $(q, \{x_\alpha\})$ space:



(a) η = 0$\Longrightarrow$ c_α=0 : escape straight along q-axis, no effect of bath.

(b) $\eta \neq$ O $\Longrightarrow$ $c_\alpha \neq$ O: escape through S

Critical point: in presence of coupling $-q\sum_\alpha C_\alpha x_\alpha - C.T.,$

saddlepoint S is shifted off q-axis, but occurs at same value of q and has same height as in absence of coupling. Now,

Gibbs-Arrhenius exponent = $V_O/k_BT,$ i.e. function only of height of S.

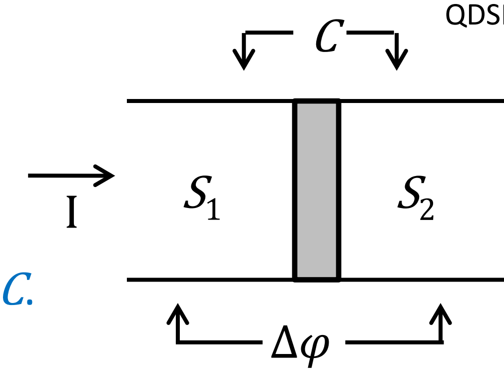
WKB exponent = $\int\sqrt{2\,mV(x)}dx/\hbar \sim \sqrt{V_O\ell}$ ← length of path to S.

V_O is unaffected by η, but ℓ is increased

$\Longrightarrow$GA exponent unchanged, WKB exponent increased!

(seems consistent with experiments on Josephson junctions)

$C\,L$ result can be applied to current-biased Josephson junction ("phase qubit") provided
$q \to \Delta\varphi \leftarrow$ C. pair phase drop
and particle "mass" → capacitance C.



But some problems:

(a) Is it legitimate to start from classical equation of motion of $\Delta\varphi(t)$ (whose whole meaning is quantum mechanical) and "re-quantize"? ("Can we quantize the equations of mathemathical economics?")

(b) Not everyone happy about insertion "by hand" of counter term.

Ambegaokar, Eckern, Schön (1982):

Consider fully microscropic model of CBJ, with bulk and tunnelling Hamiltonians expressed in terms of fermion operators $\psi(x)$.
Use HS transformation to eliminate ψ's in terms of gap (order) parameters Δ_1, Δ_2: df $\Delta\varphi \equiv \arg(\Delta_1/\Delta_2)$ ... Then express extra term in action in terms of $\Delta\varphi(t)$:

$$\Delta S \sim \iint d\tau\, d\tau' \alpha(\tau-\tau') sin^2[\Delta\,\varphi(\tau) - \Delta\varphi(\tau')]$$

$$\alpha(\tau-\tau') \propto (\tau-\tau')^{-2} \text{ for } |\tau-\tau'| \to \infty.$$

For $\Delta\varphi(\tau) \to 0$, recover osciliator-bath result, but more general.
(as it must be: $\Delta\varphi$ is periodic with period 2π)

Suggests that in general may be necessary to generalize FV scheme by

$$-q \sum_\alpha C_\alpha x_\alpha \to -f(q) \sum_\alpha C_\alpha x_\alpha$$

HOW GENERAL IS OSCILLATOR-BATH MODEL ?

Any environment E such that any one degree of freedom is only weakly perturbed by the motion of the system S can be mapped, at T=0 on to a set of SHO's, simply by associating each DOF with a separate SHO. Then quite generally

$$\hat{H}_S \rightarrow \sum_\alpha \left(p_\alpha^2/2m_\alpha + \frac{1}{2}\, m_\alpha \omega_\alpha^2 x_\alpha^2 \right)$$

$$\hat{H}_{SE} \rightarrow \sum_\alpha \{ x_\alpha F_\alpha(q,p) + p_\alpha G_\alpha(q,p) \}$$

and can integrate out oscillators exactly to get

$$S_{eff} \equiv S(q,\dot{q}:\{F_\alpha(q,\dot{q}), G_\alpha(q,\dot{q})\})$$

but resulting formula may be extremely messy and nonintuitive. Special case: adiabatic (Born-Oppenheimer) approximation. In this case,

$$S_{eff} \equiv S(q,\dot{q}:\{F_\alpha(q)\})$$

In this case, correction to uncoupled action is

$$\Delta S[q(\tau)] \sim \sum_\alpha \frac{\left[F_\alpha(q(\tau)) - F_\alpha(q(\tau'))\right]^2}{(\tau-\tau')^2}$$

while classical energy dissipation is

$$\dot{W}[q(\tau)] \sim \sum_\alpha \left(\frac{\partial F_\alpha}{\partial q}\right)^2 \dot{q}^2(\tau)$$

Hence, the "naïve" formula ($\Delta S \sim \eta\, q^{2/} \hbar$) always overestimates the effect of friction on quantum effects (e.g. tunnelling out of metastable well).

↑: justification for $\mathbf{T} \neq \mathbf{0}$?

A possibly-not-too-well-known consequence of the OB model:

FV approach with simple bilinear coupling, i.e.

$$\hat{H} = \frac{p^2}{2m} + V(q) + (SHO's) - q\sum_{\alpha} C_\alpha x_a - C.T.$$

Standard FV result for (real-time) influence functional :

$I\{q(t), q'(t)\} =$

$$exp - \frac{1}{\hbar}\int_{t_i}^{t_f} dt \int_{t_i}^{t} ds\,\{-iL_1(t-s)[q(t)-q'(t)]\cdot\big(q(s)+q'(s)\big)\}$$

$$+L_2(t-s)\{\big(q(t)-q'(t)\big)\big(q(s)-q'(s)\big)\}$$

$$L_1(t) \equiv \int_0^\infty d\omega J(\omega)\sin\omega t$$

$$L_2(t) \equiv \int_0^\infty d\omega J(\omega)\cos\omega t \;\; coth\, \beta tr\omega/2$$

spectral density

For white noise ($J(\omega) = \eta\omega$) this gives a transition amplitude in terms of

$$x(t) \equiv \frac{1}{2}\big(q(t) + q(t')\big)$$

$$y(t) \equiv q(t) - q(t')$$

of the form

$$K(q_i \to q_f)$$

$$= \int \mathcal{D}x(t) \int \mathcal{D}y(t) \exp\frac{i}{\hbar}\left\{S_o\left(x(t) + \frac{1}{2}y(t)\right)\right.$$

$$\left. - S_o\left(x(t) - \frac{1}{2}y(t)\right) - \eta\int_{t_i}^{e_f} x(t)y(t)dt\right\}$$

Phase of integral stationary for

$$M\ddot{X} + \eta\dot{X} + \partial V/\partial x = 0$$

classical damped equation of motion

In high-temperature, semiclassical limit can integrate out $y(t)$ to obtain

$$K[X(t)] \equiv \int \mathcal{D}X(t) exp - \int \{M\ddot{X} + \eta\dot{X} + \partial V/\partial X\}^2 /\eta k_B T$$

Note no reference to $\hbar$! Good starting point for classical Brownian motion.

THE AWKWARD CASE: "SATURATION" OF ENVIRONMENTAL DECREES OF FREEDOM

If the condition that any one DOF of the environment E is only weakly excited breaks down, life may become more complicated. In some cases this situation can be handled by the Born-Oppenheimer technique, but we still have to make the assumption with respect to the BO basis. What if even that breaks down?

One clear case of such breakdown appears to be a single electron spin interacting with a small number of nuclear spins even in the BO basis the nuclear spins may be highly excited. This specific case can be handled with apparent success by the "spin bath" technique of Prokofiev & Stamp (2000), but the latter appears to be much less generic than the oscillator –bath model. So, some important questions:

(1) Does there exist a technique of full generality to treat an environment whose single DOF's are strongly perturbed?
(2) In the general case, does there exist an inequality relating the quantum effects of the environment to the classical dissipation? In particular,
(3) In the general case, can we derive quantitative relations between decoherance and dissipation as we can within the OB model?

(I wish I knew……)

Happy birthday, Uli !