Breakdown of quantum-to-classical correspondence for diffusion in high temperature thermal environment

IPS 2021

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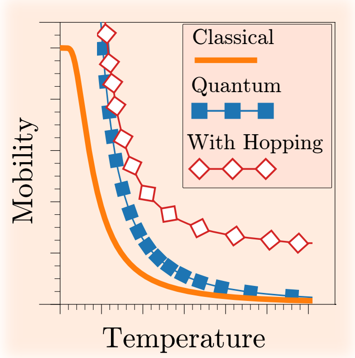


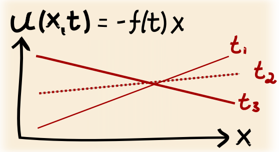
[1] DS and D. Cohen, Phys. Rev. Research 3, 013141 (2021)
[2] DS and D. Cohen, Sci. Rep. 10, 10353 (2020)

Classical Particle in a High Temperature Environment

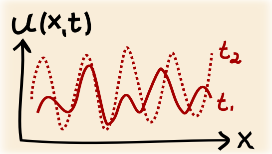
Thermal noise: $f = -\partial_x \mathcal{U}(x,t)$ [$\mathcal{U}(x,t)$ Fluctuating potential]

ν is the noise intensity [ℓ Spatial Correlation]

$\ell = \infty$ (Caldeira-Leggett)



$\ell = a =$ lattice constant



Same Langevin equation: $\dot{p} \; = \; -\eta \dot{x} + f$

Friction: $\eta = \nu / 2T$ [T = Temperature]

Diffusion and mobility ($\dot{x} = p/m$)**:** $D = \dfrac{T}{\eta} \qquad \mu = \dfrac{1}{\eta}$

Quantum ?

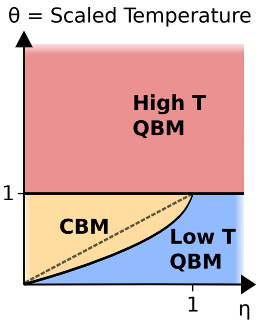
Quantum Signature in High Temperature

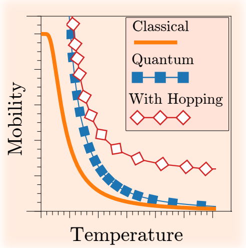
We look for quantum mechanical signature in a high temperature system.
(Ohmic master equation: $\dot{\rho} = \mathcal{L}\rho$)

- Caldeira-Leggett ($\ell = \infty$):
  Dynamics is the same as classical.
  Same D, μ.

- Finite ℓ:
  Common wisdom – same transport coefficients.

  Our statement:
  D, μ depend on ℓ even at high temperature.





ℓ = Spatial correlation of the environment $\qquad \eta$ = Friction coefficient

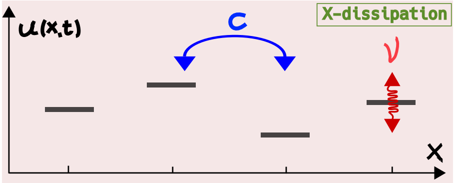
Model: Tight-binding + coupling to the environment

$\boldsymbol{H}_0 = -\boldsymbol{c}\cos(a\hat{\boldsymbol{p}})$ $\qquad$ [$a = 1$]

Coupling Terms:

X-dissipation: $\boldsymbol{H}^{(\text{int})} = -f(t)\,\boldsymbol{x}$ $\qquad$ [$\ell = \infty$, Caldeira-Leggett]

S-dissipation: $\boldsymbol{H}^{(\text{int})} = -\sum_x f_x(t)|\boldsymbol{x}\rangle\langle\boldsymbol{x}|$ $\qquad$ [$\ell = a = 1$]



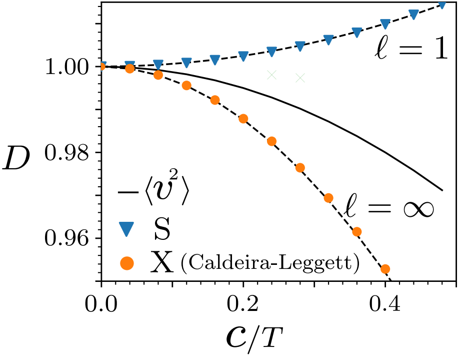
Ohmic master equation: $\frac{d\rho}{dt} = \mathcal{L}\rho = -i[\boldsymbol{H}_0, \rho] + \mathcal{L}^{(\text{bath})}\rho$

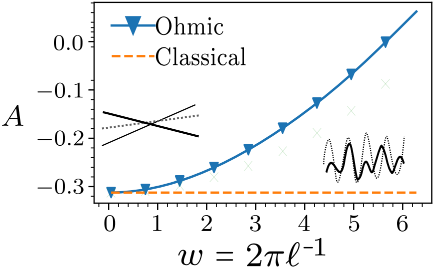
Parameters: **c**, $\boldsymbol{\nu}$, $\boldsymbol{\eta}$.

$$\boldsymbol{H}^{(\text{int})} = -f_\alpha \boldsymbol{W}_\alpha \Rightarrow \mathcal{L}_\alpha = \frac{\nu}{2}[\boldsymbol{W}_\alpha, [\boldsymbol{W}_\alpha, \rho]] + \frac{\eta}{2}\, i[\boldsymbol{W}_\alpha, \{\boldsymbol{V}_\alpha, \rho\}]$$

$$\boldsymbol{V}_\alpha \equiv i[\boldsymbol{H}_0, \boldsymbol{W}_\alpha]$$

Diffusion: $D \propto \left[1 + A\left(\frac{c}{T}\right)^2\right]\frac{c^2}{\nu}$





$$A = \begin{cases} -5/16 & \text{X-coupling } (l{=}\infty) \\ +1/16 & \text{S-coupling } (l{=}1) \\ -1/8 & \langle v^2\rangle \end{cases}$$

General ℓ:

$$A \approx -\frac{5}{16}\left(1 - \frac{6}{5}\left(\frac{a}{\ell}\right)^2\right)$$

Parameters: Noise intensity ν is fixed. Varying temperature T. Hopping frequency **c**

X-coupling

Same diffusion coefficient for classical and quantum system.

Classical equations with an added field f_0:

$$\dot{x} = \frac{\partial H}{\partial p} = c \sin(p)$$

$$\dot{p} = -\frac{\partial H}{\partial x} = f_0 - \eta \dot{x} + f(t)$$

Fokker-Planck equation for momentum: $\dot{\rho}(p) = -\frac{d}{dp} J$ [J = p current]

Obtain Steady state: $\rho_{ss}(p)$

Extract mobility:

$$\langle \dot{x} \rangle_{ss} = \left[1 - \mathrm{I}_0^{-2}\left(\frac{c}{T}\right)\right] \frac{f_0}{\eta} \equiv \mu f_0$$

Use Einstein relation: $D = \mu T$.

The solution is “good” for all T (provided the Ohmic master equation holds).

Obtain the diffusion

Master equation: $\frac{d\rho}{dt} \;=\; \mathcal{L}\rho \;=\; -i[\boldsymbol{H}_0, \rho] + \mathcal{L}^{(\text{bath})}\rho$

Eigenvalues: $\mathcal{L}\rho = -\lambda\rho$

Standard representation: $\rho(R, r) \equiv \langle R + r/2|\rho|R - r/2\rangle$

Bloch representation: $\rho(q; r)$ [q is a constant of motion]

Eigenvalues: $\lambda_{q,0} \;=\; Dq^2 + \mathcal{O}(q^4)$ [Lowest band]

Obtain D: Perturbation theory in q and η

Example. $\mathcal{L}^{(q)}_{r'',r'}$ (X-coupling):

$$\mathcal{L}^{(q)} \mapsto \frac{1}{2}\begin{pmatrix} -4\nu & 2c\eta{-}cq & 0 & 0 & 0 \\ -c\eta{+}cq & -\nu & c\eta{-}cq & 0 & 0 \\ 0 & cq & 0 & -cq & 0 \\ 0 & 0 & c\eta{+}cq & -\nu & -c\eta{-}cq \\ 0 & 0 & 0 & 2c\eta{+}cq & -4\nu \end{pmatrix}$$

Quantum analysis (Wigner representation)

We obtain an “exact” stochastic equation: With the same D (to order T^{-2}).

Wigner representation: $\rho(R, r) \to \rho(R, P)$.

Stochastic-like kernel ($\eta = 0$):

$$\mathcal{L}^{(\text{bath})}(R, P|R_0, P_0) = \mathcal{W}(P|P_0)\delta(R - R_0)$$

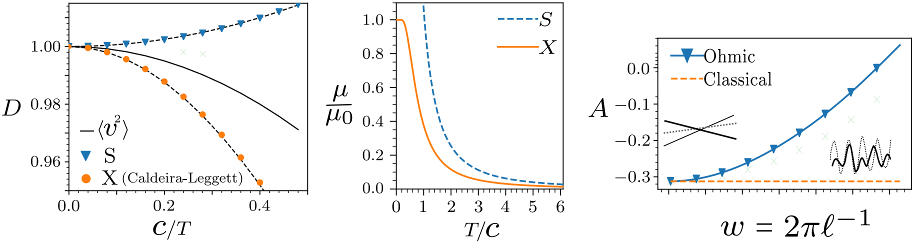
$$\mathcal{W}(P|P_0) = \begin{cases} \left(\frac{L}{2\pi}\right)^2 \frac{\nu}{2}\delta_{P,P_0\pm(2\pi/L)} & \text{, X-coupling} \\ \left(\frac{\nu}{L}\right) & \text{, S-coupling} \end{cases}$$

At finite temperature:

$$\mathcal{W} \mapsto \mathcal{W} \exp\left[-\frac{E(P)-E(P_0)}{2T}\right] \qquad [\ E(P) = -c\cos(P)\ ]$$

Summary

- Diffusion in high temperature environment has quantum fingerprints.
- The coefficient A is non-universal, and depends on ℓ.
- Underlying mechanism for dissipation is reflected.
- More results in [2] regarding the effects of disorder.



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