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

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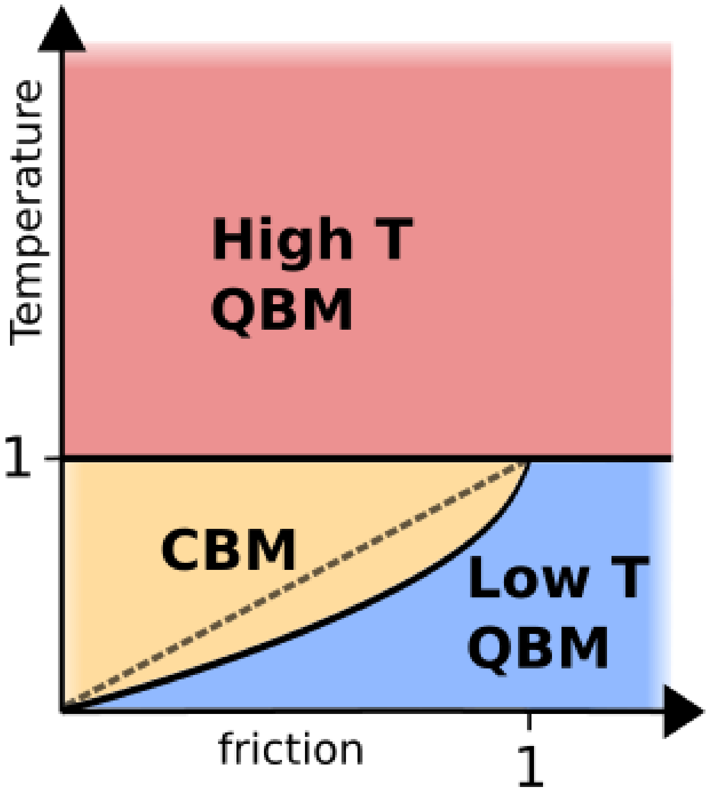
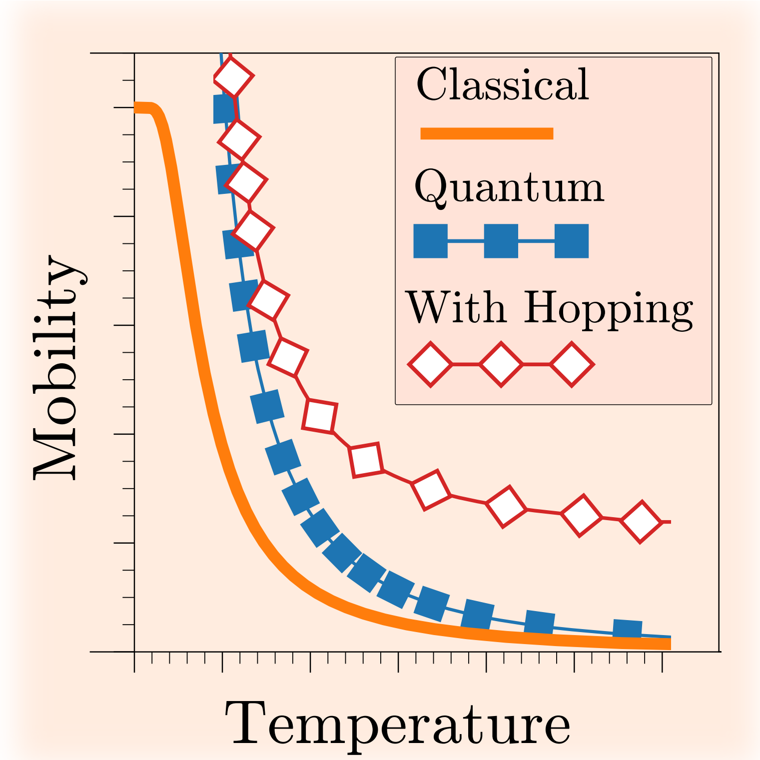
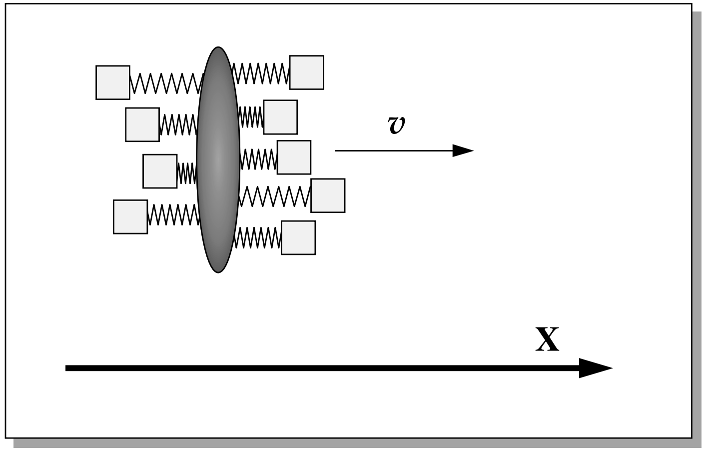
[1] Dekel Shapira, DC, Phys. Rev. Research 3, 013141 (2021).

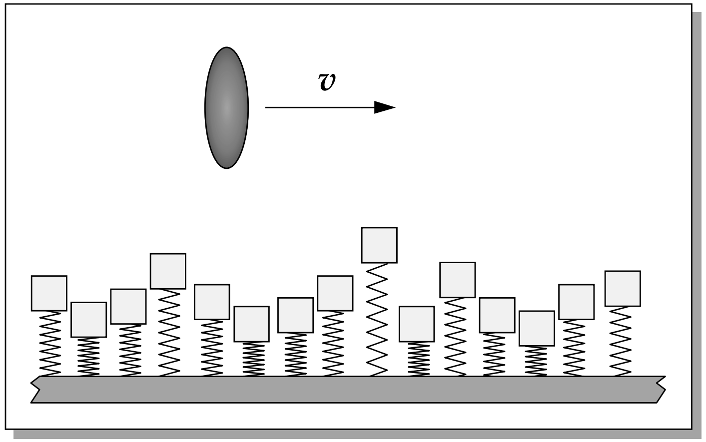
[2] Dekel Shapira, DC, Sci. Rep. 10, 10353 (2020).





Brownian motion: Beyond Caldeira-Leggett





$$\dot{p} \;=\; -\eta\dot{x} + f$$

$$\mathcal{H}_{total} \;=\; \mathcal{H}_0(\boldsymbol{x},\boldsymbol{p}) \;+\; \mathcal{H}_{\mathrm{bath}}(Q,P) \;+\; \mathcal{H}_{X/S}$$

$$\mathcal{H}_0(\boldsymbol{x},\boldsymbol{p}) \;=\; \frac{1}{2M}\boldsymbol{p}^2 + V_0(\boldsymbol{x}) \;-\; f_0\boldsymbol{x}$$

$$\mathcal{H}_{\mathrm{bath}} = \sum_{\alpha}\left(\frac{{P_\alpha}^2}{2\mathsf{m}_\alpha} + \frac{1}{2}\mathsf{m}_\alpha\omega_\alpha^2{Q_\alpha}^2\right)$$

An $\ell = \infty$ environment:

$$\mathcal{H}_{\mathrm{X}} \;=\; -\boldsymbol{x}\sum_{\alpha} c_\alpha Q_\alpha$$

A finite ℓ environment

$$\mathcal{H}_{\mathrm{S}} \;=\; -\sum_{\alpha} c_\alpha Q_\alpha u(\boldsymbol{x}-x_\alpha)$$

Thermal stochastic potential:

$$f \;=\; -\partial_x\mathcal{U}(x,t)$$

Spatial correlation scale ℓ

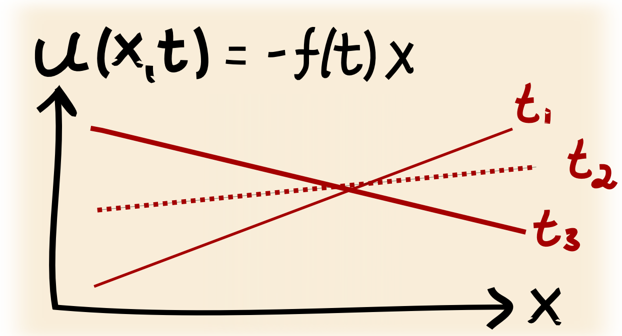
[DC, Phys Rev E (1997); Phys Rev Lett (1997)]

Brownian motion

The stochastic potential $\mathcal{U}(x,t)$ features in general a spatial correlation scale ℓ.
In the Caldeira-Leggett model f is independent of x, meaning that $\ell = \infty$.
The transport coefficients do not depend on ℓ.

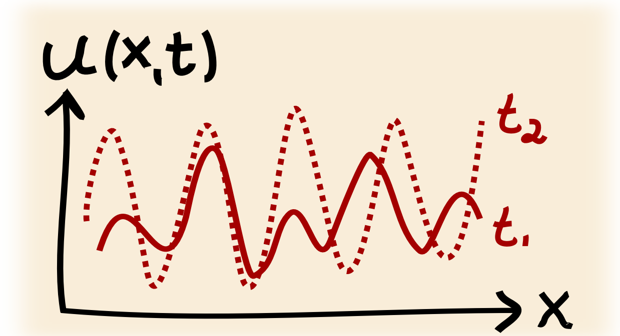
$$\begin{aligned} \dot{p} &= -\eta\dot{x} + f \\ f &= -\partial_x \mathcal{U}(x,t) \end{aligned}$$

We assume high temperature Ohmic bath



Model parameters:

$$\begin{aligned} \nu &= \text{noise intensity} \\ \eta &= \frac{\nu}{2T} = \text{friction coefficient} \end{aligned}$$



Transport coefficient (same for Quantum and for Classical):

$$\begin{aligned} \mu &= \frac{1}{\eta}, \qquad [\text{mobility}] \\ D &= \frac{\nu}{2\eta^2}, \qquad [\text{diffusion coefficient}] \end{aligned}$$

Ratio satisfies Einstein relation

ℓ does not affect
the classical dynamics
and has no signature
in transport coefficients.

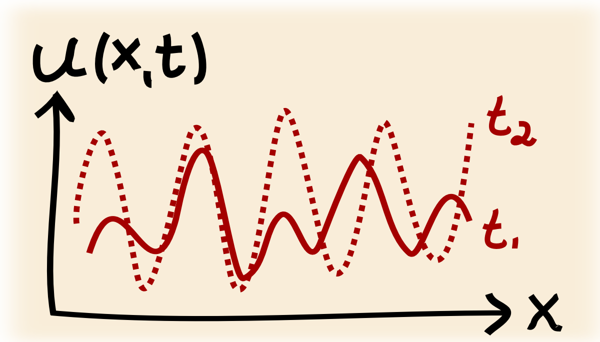
Quantum signature of ℓ

ℓ determines the lineshape of the stochastic kernel $\mathcal{W}(k|k')$ for scattering from k' to k.
The quantum mechanical width of the kernel is $\sim 2\pi\hbar/\ell$.
Its second moment is ν.
It has implication on the decoherence process (short time transient).
It has no implication on the transport coefficients (central limit theorem).

Quantum decoherence rate:

$$\left(\frac{1}{\tau_\varphi}\right)_X = \frac{\nu L^2}{\hbar^2} \qquad [L \text{ is e.g. distance between the slits}]$$

$$\left(\frac{1}{\tau_\varphi}\right)_S = \frac{\nu \ell^2}{\hbar^2} \qquad [\ell \text{ is the spatial correlation scale}]$$



Extension to low temperatures:

[1] DC, J. Phys. A (1998).
[2] DC, Y. Imry, Phys. Rev. B (1999).
[3] D.C, J. von Delft, F. Marquardt, Y. Imry, Phys. Rev. B (2009).

$$\text{Width}\Big[\mathcal{W}(k|k')\Big] = \frac{2\pi\hbar}{\ell}$$

$$\sum_k \mathcal{W}(k|k')(k-k')^2 = \nu$$

Tight binding model

$$\boldsymbol{H}_0 \;=\; -c\cos(a\boldsymbol{p}) - f_0\boldsymbol{x}, \qquad [a=1], \qquad \cos(\boldsymbol{p}) = \frac{1}{2}\sum_x \Big[\,|x{+}1\rangle\langle x| + |x\rangle\langle x{+}1|\,\Big]$$

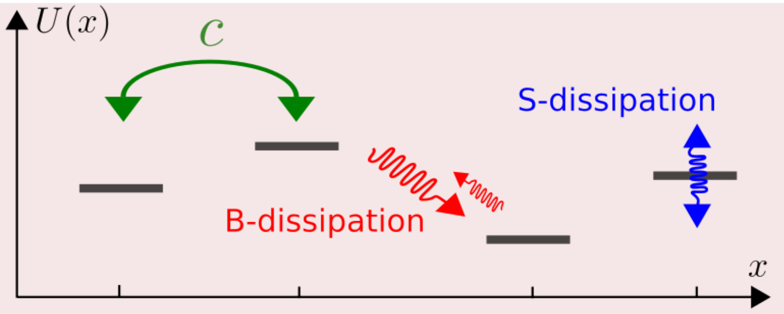
$$\alpha \;=\; \frac{\eta a^2}{2\pi} \;=\; \text{dimensionless friction} \qquad\qquad v_{\text{drift}} \;=\; \mu\ f_0$$

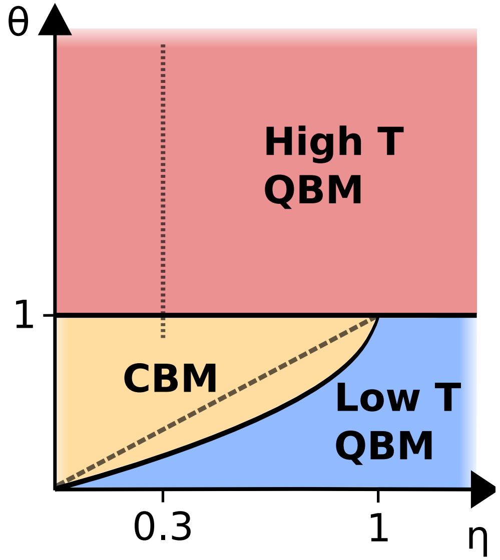
$$\theta \;=\; \frac{T}{c} \;=\; \text{dimensionless temperature} \qquad\qquad \mu^{(\text{cl})} \;=\; \left[1 - \frac{1}{[\mathbf{I}_0(1/\theta)]^2}\right]\frac{1}{\eta}$$

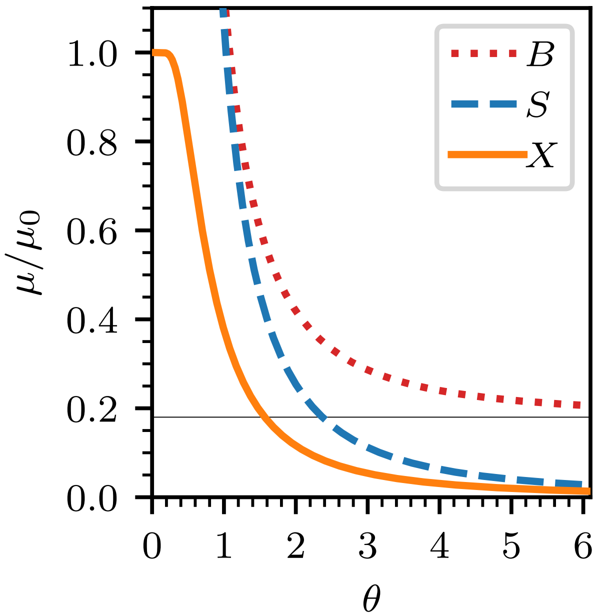
X: fluctuating homogeneous field with ($\ell = \infty$)

S: site dissipation - fluctuating potential ($\ell = a$)

B: bond dissipation - thermally induced hopping







Low temperature regime analysed e.g. by C. Aslangul, N. Pottier, D. Saint-James, Journal de Physique (1986).

Further motivation comes from recent studies of transport in photosynthetic light-harvesting complexes.

For a detailed list of references see DS and DC, Phys. Rev. Research (2021).

The Ohmic master equation

The dynamics is described by an Ohmic master equation (i.e. high temperature approximation):

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

The interaction with the bath is written as

$$\mathcal{H}_{\mathrm{interaction}} = -\sum_{\alpha} \boldsymbol{W}_\alpha F_\alpha$$

One defines generalized "velocity" operators:

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

The Ohmic dissipator is:

$$\mathcal{L}^{(\mathrm{bath})}\rho = -\sum_{\alpha}\left(\frac{\nu}{2}[\boldsymbol{W}_\alpha,[\boldsymbol{W}_\alpha,\rho]] + \frac{\eta}{2}\, i[\boldsymbol{W}_\alpha,\{\boldsymbol{V}_\alpha,\rho\}]\right)$$

Spectrum:

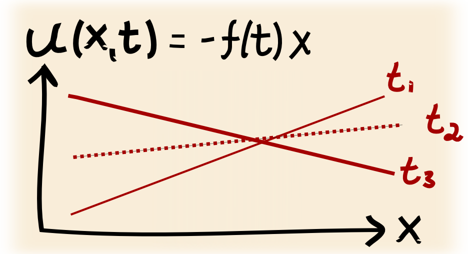
$$\mathcal{L}\rho = -\lambda\rho$$

$$\rightsquigarrow \quad \lambda_{q,s}, \quad s = 0, \pm1, \pm2, \ldots$$

$$\lambda_{q,0} = ivq + Dq^2 + \mathcal{O}(q^3)$$

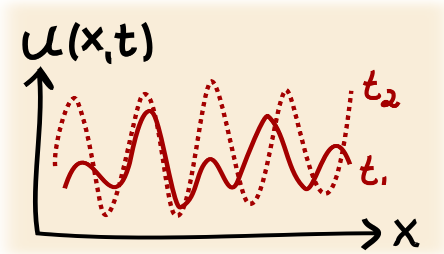
For X-dissipation:

$$\boldsymbol{W} = \boldsymbol{x}$$
$$\boldsymbol{V} = \frac{1}{M}\boldsymbol{p}$$



For S-dissipation:

$$\boldsymbol{W}_\alpha = |x_\alpha\rangle\langle x_\alpha|$$



The Bloch representation

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

Bloch representation: $\rho(R,r) \;\rightsquigarrow\; \rho(q;r)$

$$
\begin{aligned}
\mathcal{L}^{(c)} &= +\sin(q/2)\Big(\mathcal{D}_\perp - \mathcal{D}_\perp^\dagger\Big) \\
\mathcal{L}^{(\nu_X)} &= -(1/2)\hat{r}^2 \\
\mathcal{L}^{(\eta_X)} &= \cos\,(q/2)\frac{\hat{r}}{2}\Big(D_\perp - D_\perp^\dagger\Big) \\
\mathcal{L}^{(\nu_S)} &= -1 + 1\,|0\rangle\langle 0| \\
\mathcal{L}^{(\eta_S)} &= \frac{\cos\,(q/2)}{2}\Big(\mathcal{D}_\perp + D_\perp^\dagger + |\pm1\rangle\langle 0| - |0\rangle\langle\pm1|\,\Big) \\
\mathcal{L}^{(\nu_B)} &= -2 \;+\; 2\cos(q)\,|0\rangle\langle 0| + \Big(\,|1\rangle\langle -1| + |-1\rangle\langle 1|\,\Big) \\
\mathcal{L}^{(\eta_B)} &= \frac{1}{2}\cos\,(q/2)\Big(\mathcal{D}_\perp + \mathcal{D}_\perp^\dagger\Big) \\
&+ \frac{1}{2}\cos(3q/2)\Big(\,|\pm1\rangle\langle 0| - |0\rangle\langle\pm1|\,\Big) \\
&+ \frac{1}{2}\cos(q/2)\Big(\,|\mp2\rangle\langle\pm1| - |\pm1\rangle\langle\mp2|\,\Big)
\end{aligned}
$$

$$\mathcal{D}_\perp = \sum_r |r{+}1\rangle\langle r|$$

Results for the transport coefficients

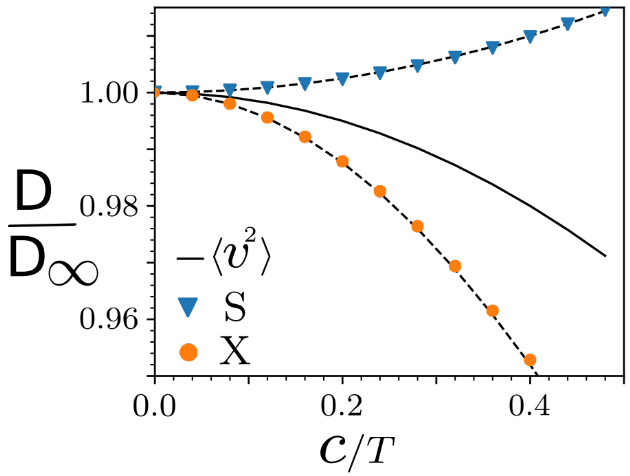
The exact classical result:

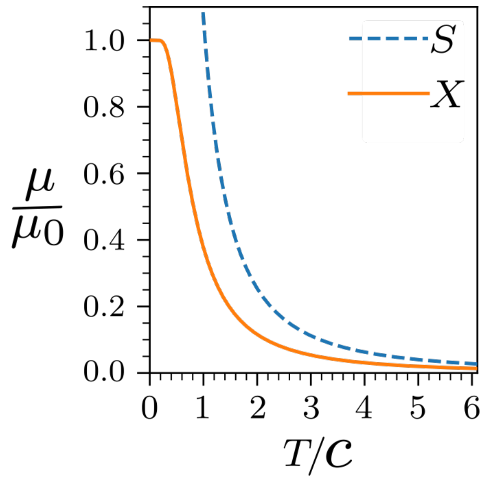
$$D^{(\mathrm{X})} \ = \ \left[1 - \frac{1}{[\mathrm{I}_0(c/T)]^2}\right] \frac{T}{\eta}$$

Formal hight temperature expansion:

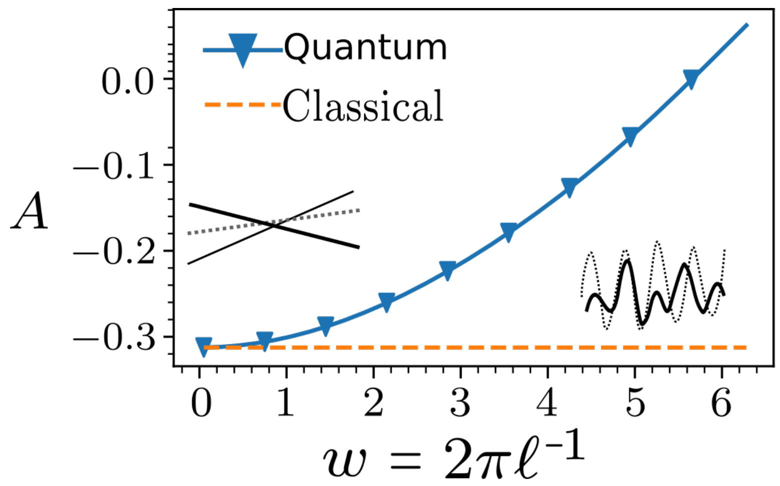
$$D \ \approx \ \left[1 + A\left(\frac{c}{T}\right)^2\right] \frac{c^2}{\nu}$$

$$\langle v^2 \rangle \ \approx \ \left[1 + A\left(\frac{c}{T}\right)^2\right] \frac{c^2}{2}$$





$$A \ = \ \begin{cases} -1/8 & \text{for } \langle v^2 \rangle \\ -5/16 & \text{for X-dissipation} \\ +1/16 & \text{for S-dissipation} \\ -\frac{5}{16}\left(1 - \frac{6}{5}\left(\frac{a}{\ell}\right)^2\right) & \text{general } \ell \end{cases}$$



In the $D(T)$ figure $D_\infty = c^2/\nu$ is fixed.

In the $\mu(T)$ figure $\mu_0 = 1/\eta$ is fixed.

Effective stochastic picture

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

Wigner representation: $\rho(R,r) \;\rightsquigarrow\; \rho_w(R,P)$

We obtain an "exact" stochastic approximation for the time evolution of Wigner function.
It is "exact" in the sense that it features the same D to order T^{-2}.

Stochastic-like kernel:

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

$$\mathrm{Width}\Big[\mathcal{W}(k|k')\Big] \;=\; \frac{2\pi\hbar}{\ell}$$

$$\sum_k \mathcal{W}(k|k')(k-k')^2 \;=\; \nu$$

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

At finite temperature:

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

$$E(P) = -c\cos(P)$$

Introduction of disorder

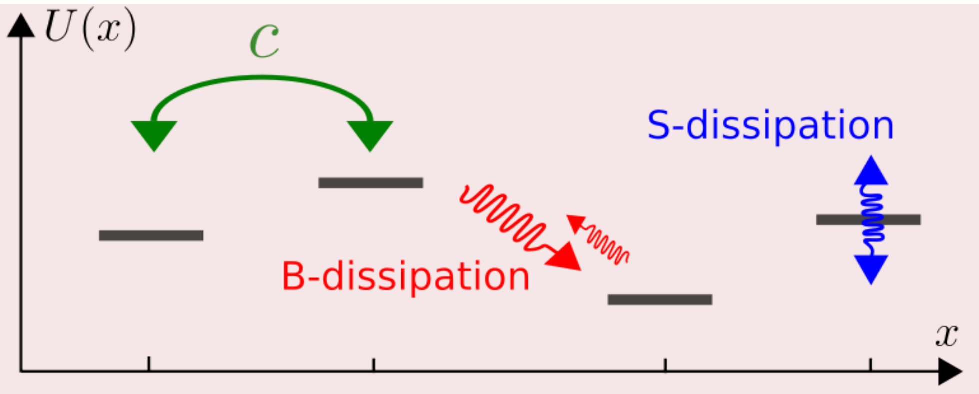
Quantum version of Sinai-Derrida-Hatano-Nelson model.

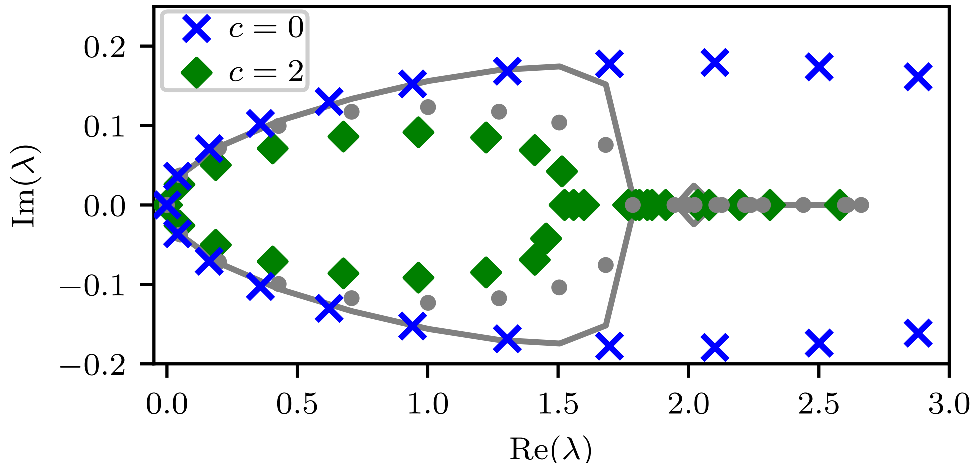
A quantum analysis of *random walk in random environment*.

Due to disorder (random transition rates) diffusion is suppressed.

We ask: what would be the result if we have both coherent and stochastic transitions *in parallel*.

We find: counter-intuitive enhancement of the effective disorder due to coherent hopping.

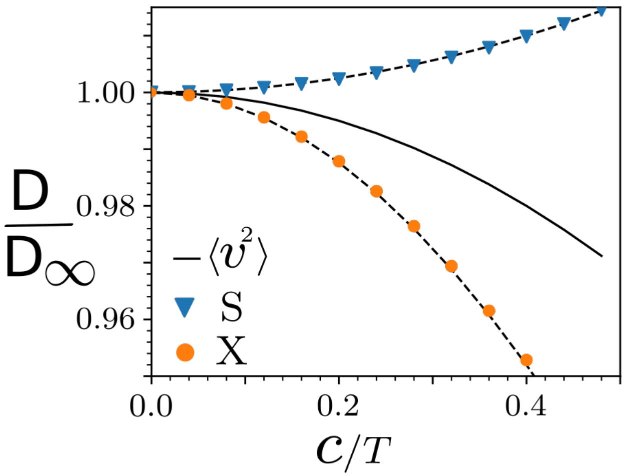


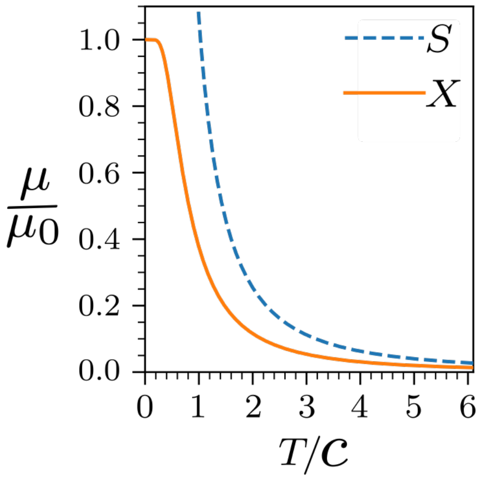


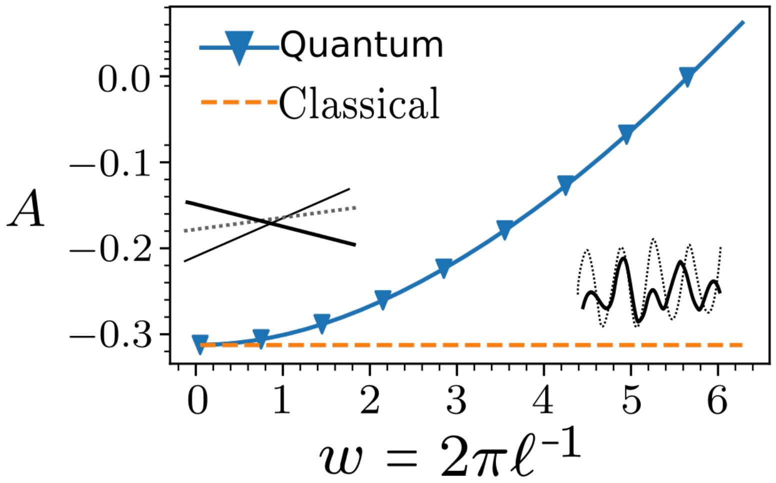
Recall: for normal diffusive system $\lambda_q \;=\; ivq + Dq^2 + \mathcal{O}(q^3)$

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 due to disorder.







[1] Dekel Shapira, DC, Phys. Rev. Research 3, 013141 (2021).

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