Thermodynamic Uncertainty Relation in Markovian and Non-Markovian Regimes

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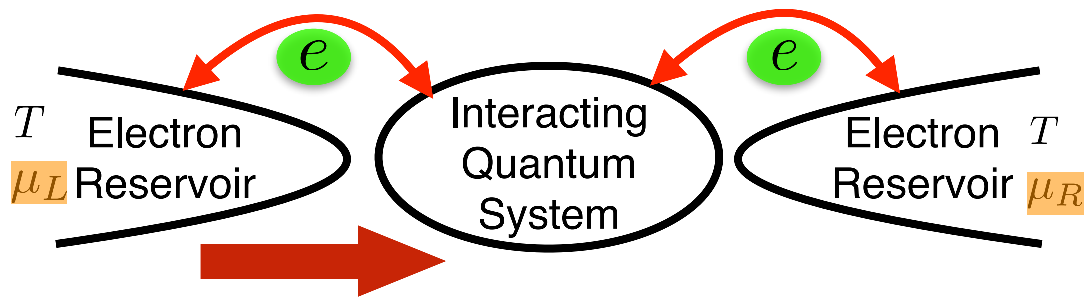
Fundamental aspects of non-equilibrium statistical physics

Linear Irreversible Thermodynamics

Linear response theory: Summarized via **universal** **Onsager's reciprocity relations**, **universal** **Fluctuation-dissipation relations**.



$$\langle j \rangle = G_1 V + \frac{1}{2!} G_2 V^2 + \frac{1}{3!} G_3 V^3 \cdots$$

$$\langle\langle j^2 \rangle\rangle = S_0 + S_1 V + \frac{1}{2!} S_2 V^2 + \frac{1}{3!} S_3 V^3 \cdots .$$

$$V = \mu_L - \mu_R$$

Johnson-Nyquist theorem

Conductance is proportional to the current noise at equilibrium

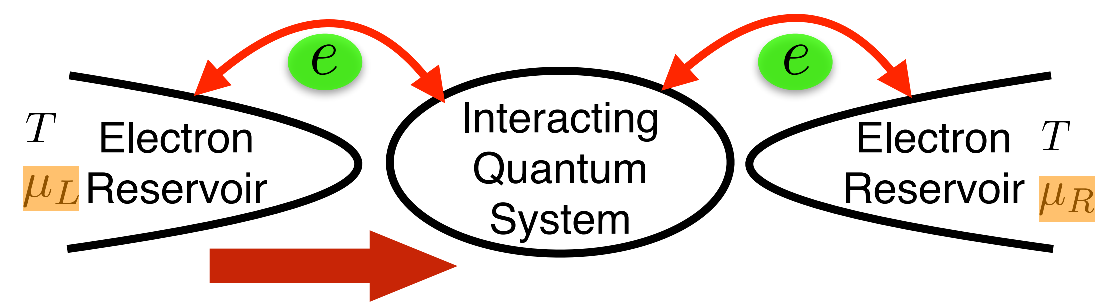
$$\boxed{S_0 = 2\, k_B\, T\, G_1}$$

What about far from equilibrium??

Fluctuation Relations: Microscopic statement of second law

- **Charge Transport**

$$n = \int I_{el}(t)dt$$ stochastic variable



$$\ln\left[\frac{P_t(+n)}{P_t(-n)}\right] = \beta\,(\mu_L - \mu_R)n$$

Gallavotti-Cohen fluctuation symmetry

- **Close to equilibrium ⟶ Standard Linear response results**
- **Response coefficients are related beyond linear response regime**

$$\langle j \rangle = G_1 V + \frac{1}{2!} G_2 V^2 + \frac{1}{3!} G_3 V^3 \cdots$$

$$\langle\langle j^2 \rangle\rangle = S_0 + S_1 V + \frac{1}{2!} S_2 V^2 + \frac{1}{3!} S_3 V^3 \cdots .$$

The steady state fluctuation symmetry ensures that

$$S_0 = 2\,k_B\,T\,G_1$$ **Fluctuation-dissipation relation (Johnson-Nyquist relation)**

$$S_1 = k_B\,T\,G_2$$ **Relation between Nonlinear Coefficients**

Recent Work

Experimental verification of quantum heat exchange fluctuation relation

Soham Pal,[1,*] T. S. Mahesh,[1,†] and Bijay Kumar Agarwalla[1,‡]

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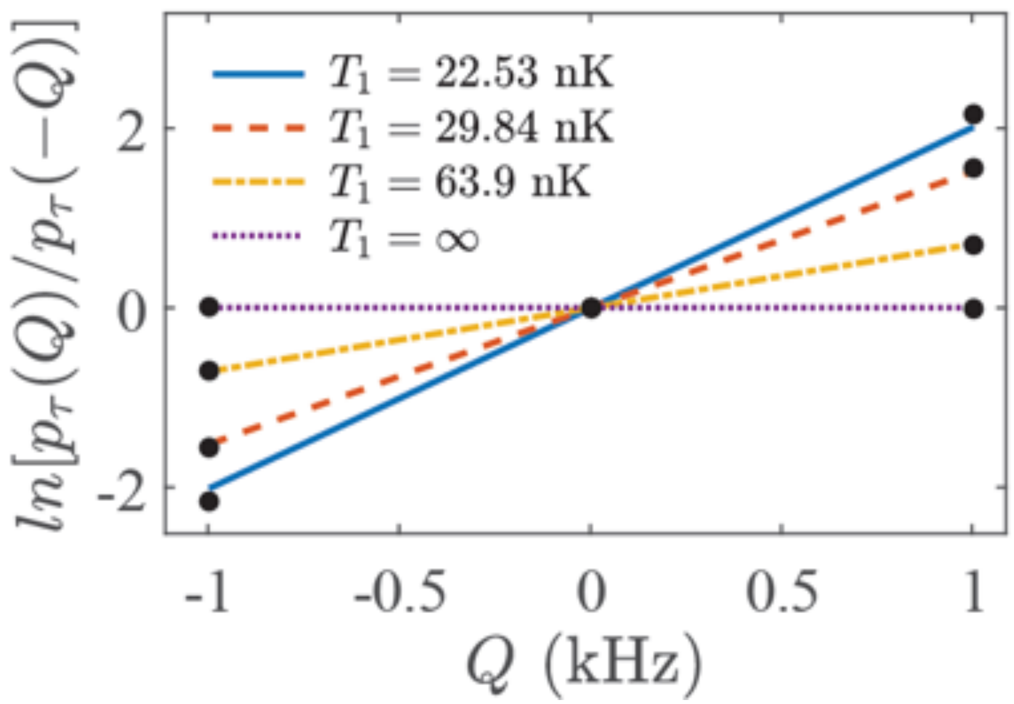
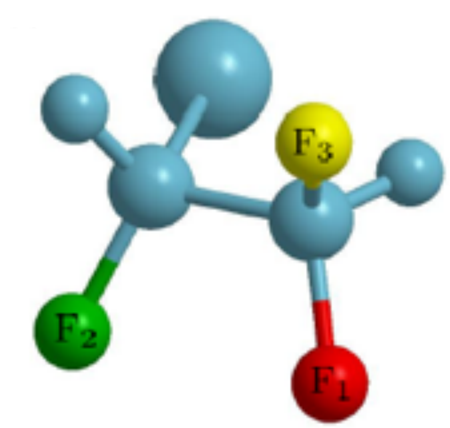
arXiv: 1811.07291



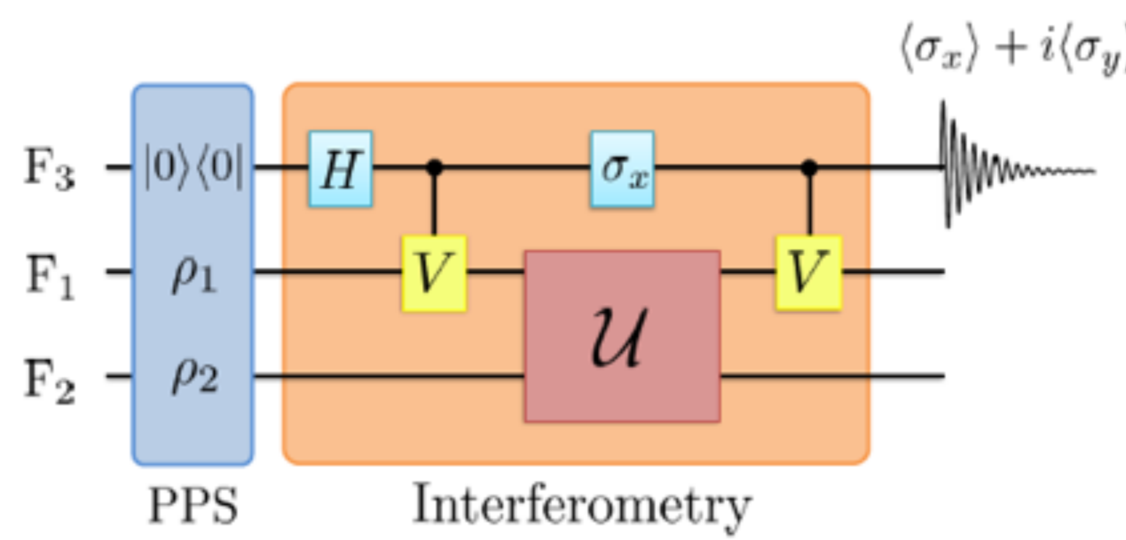
$$\ln \frac{p_\tau(Q)}{p_\tau(-Q)} = \Delta\beta Q$$



1, 1, 2–Trifluoro –2 –iodoethane

Hamiltonian Parameters

F_1(Hz)	F_2(Hz)	F_3(Hz)	
1000	−128.3	69.9	F_1(Hz)
	−16330	47.4	F_2(Hz)
		12839	F_3(Hz)



Thermodynamic Uncertainty Relation (TUR)

Trade-off between dissipation (entropy production) and precision (noise)

For two-terminal single-affinity system (Markov Process)

$$\frac{\langle\langle j^2 \rangle\rangle}{\langle j \rangle^2} \frac{\sigma}{k_B} \geq 2.$$

.. Seifert PRL (2018), PRL (2015), PRE (2016)
..England PRL (2016)

Equality in the linear response regime (Gaussian distribution)

$$\frac{\langle\langle j^2 \rangle\rangle}{\langle j \rangle^2} \frac{\sigma}{k_B} \overset{?}{\geq} 2.$$

Relation to fluctuation symmetry?
Quantum Effects?

B. K. Agarwalla, D. Segal PRB (2018)

Thermodynamic Uncertainty Relation (TUR)

Cost - precision tradeoff

$$\frac{\langle\langle j^2\rangle\rangle}{\langle j\rangle^2}\frac{\sigma}{k_B} \overset{?}{\geq} 2$$

A. C. Barato and U. Seifert, Thermodynamic uncertainty relation for biomolecular processes, Phys. Rev. Lett. **114**, 158101 (2015).

P. Pietzonka, A. C. Barato, and U. Seifert, Universal bounds on current fluctuations, Phys. Rev. E **93**, 052145 (2016).

T. R. Gingrich, J. M. Horowitz, N. Perunov, and J. L. England, Dissipation bounds all steady state current fluctuations, Phys. Rev. Lett. **116**, 120601 (2016).

Thermodynamic Uncertainty Relation (TUR): Charge Transport

$$\langle j \rangle = G_1 V + \frac{1}{2!} G_2 V^2 + \frac{1}{3!} G_3 V^3 \cdots$$

$$\langle\langle j^2 \rangle\rangle = S_0 + S_1 V + \frac{1}{2!} S_2 V^2 + \frac{1}{3!} S_3 V^3 \cdots .$$

$$\frac{\langle\langle j^2 \rangle\rangle}{\langle j \rangle^2} \frac{\sigma}{k_B} \overset{?}{\geq} 2.$$

The steady state fluctuation symmetry ensures that

$$S_0 = 2\, k_B\, T\, G_1,$$
$$S_1 = k_B\, T\, G_2 .$$

The entropy production: $\sigma = V \langle j \rangle / T$

TUR: $$\beta V \frac{\langle\langle j^2 \rangle\rangle}{\langle j \rangle} = 2 + \frac{V^2}{G_1} C_{\text{neq}} + \mathcal{O}(V^4) + \cdots$$

Sign?

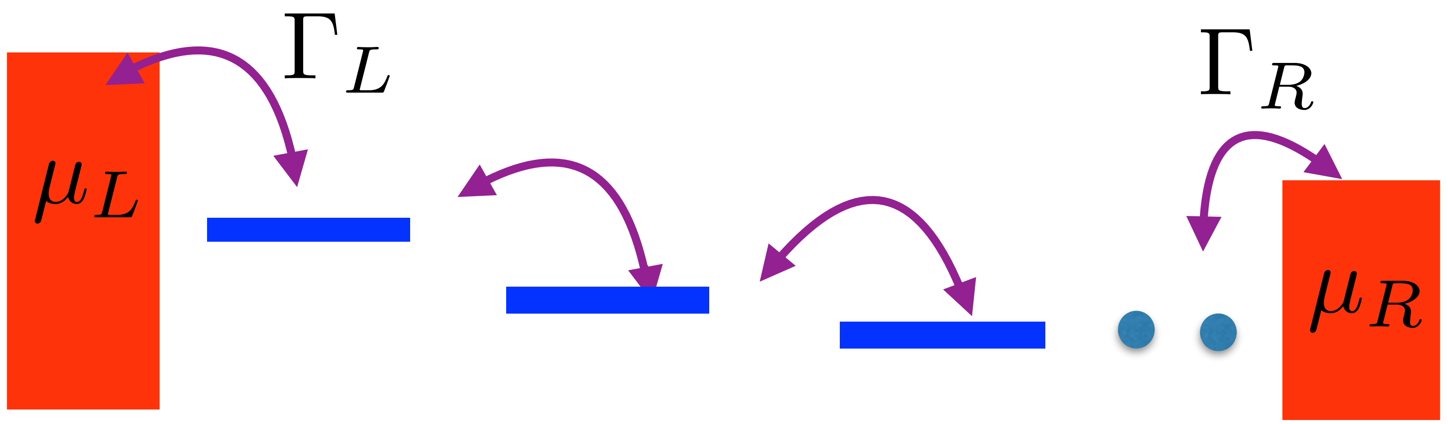
$$C_{\text{neq}} = \frac{\beta}{6} \left[3 S_2 - 2 k_B T G_3 \right].$$

nonlinear transport coefficients

Valid for both classical and quantum systems

Non-interacting Charge Transport (Scattering Theory)

Model: Tight-binding chain connected to two fermionic leads



Levitov, Lesovik (1993)
Klich (2003)
Esposito et al (2009)
Agarwalla et al (2012)

Charge Current: (Landauer Formula)

$$\langle j \rangle = \frac{\partial \chi}{\partial (i\alpha)}\Big|_{\alpha=0} = \int_{-\infty}^{\infty} \frac{dE}{2\pi\hbar} \mathcal{T}(E)\left[f_L(E) - f_R(E)\right]$$

Current Fluctuation:

$$\langle\langle j^2 \rangle\rangle = \frac{\partial^2 \chi}{\partial (i\alpha)^2}\Big|_{\alpha=0} = \int_{-\infty}^{\infty} \frac{dE}{2\pi\hbar} \Big\{ \mathcal{T}(E)\left[f_L(E)(1-f_L(E)) + f_R(E)(1-f_R(E))\right] + \mathcal{T}(E)(1-\mathcal{T}(E))(f_L(E)-f_R(E))^2 \Big\}$$

Non-interacting Charge Transport

$$\beta V \frac{\langle\langle j^2 \rangle\rangle}{\langle j \rangle} = 2 + \frac{V^2}{G_1} C_{\mathrm{neq}} + \mathcal{O}(V^4) + \cdots$$

$$C_{\mathrm{neq}} \equiv \frac{\beta^2}{6} \int_{-\infty}^{\infty} \frac{dE}{2\pi\hbar} \mathcal{T}(E) \frac{\partial f(E)}{\partial \mu} \left[1 - 6\,\mathcal{T}(E) f(E)(1 - f(E)) \right]$$

Can switch sign

1. Structure of the transmission function (tunnelling processes),
2. External conditions (temperature)

Low transmission, $\mathcal{T}(E) \ll 1$ $\quad \beta V \frac{\langle\langle j^2 \rangle\rangle}{\langle j \rangle} = 2 + \frac{\beta^2 V^2}{6}$ valid

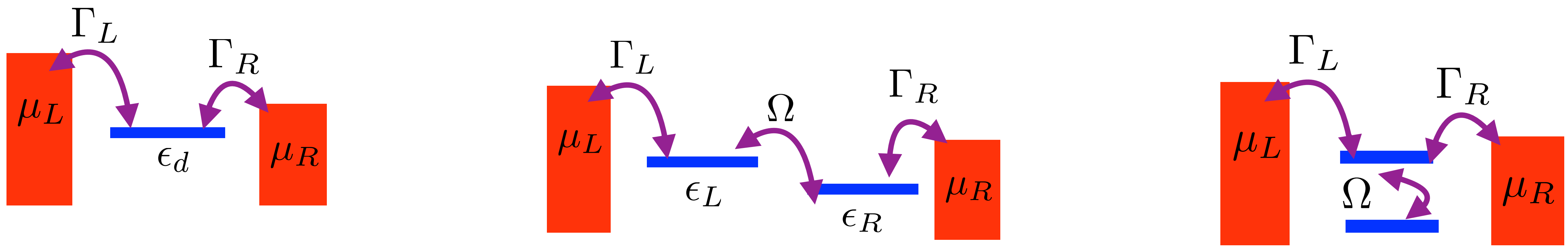
Constant Transmission $\mathcal{T}(E) = \tau$ $\quad \beta V \frac{\langle\langle j^2 \rangle\rangle}{\langle j \rangle} = 2 + \frac{\beta^2 V^2}{12\pi\hbar G_1} \tau(1 - \tau)$

valid

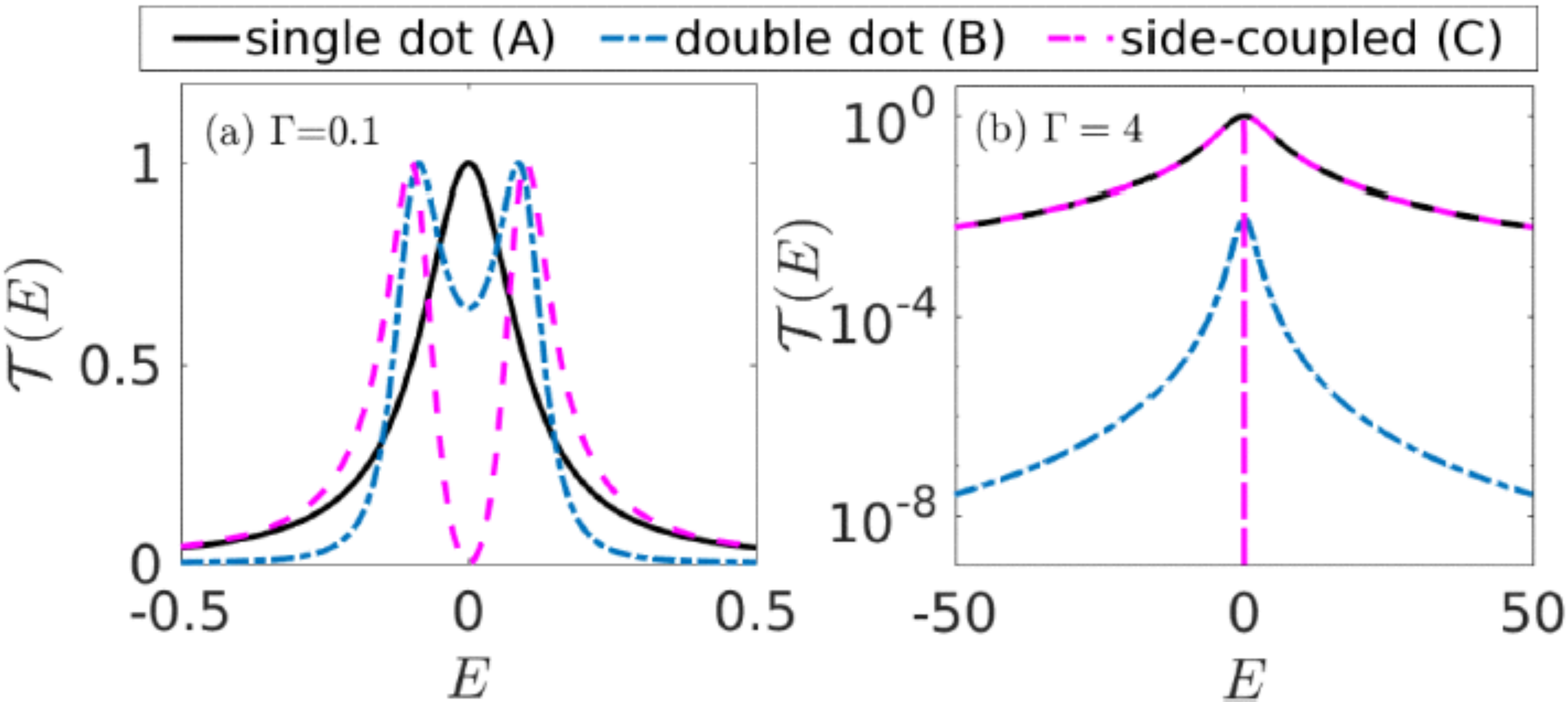
Resonance tunneling condition

Violation condition: $\frac{\mathcal{T}_2}{\mathcal{T}_1} > \frac{2}{3}$ $\quad \mathcal{T}_n \equiv \int_{-\infty}^{\infty} \frac{dE}{2\pi\hbar} \mathcal{T}^n(E)$

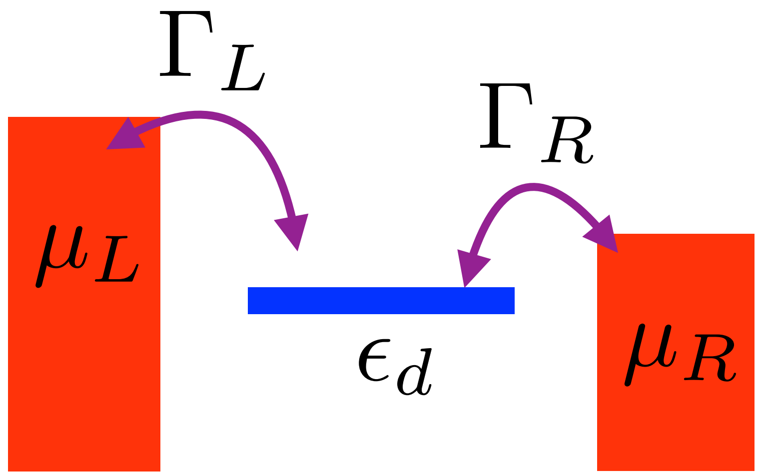
Examples



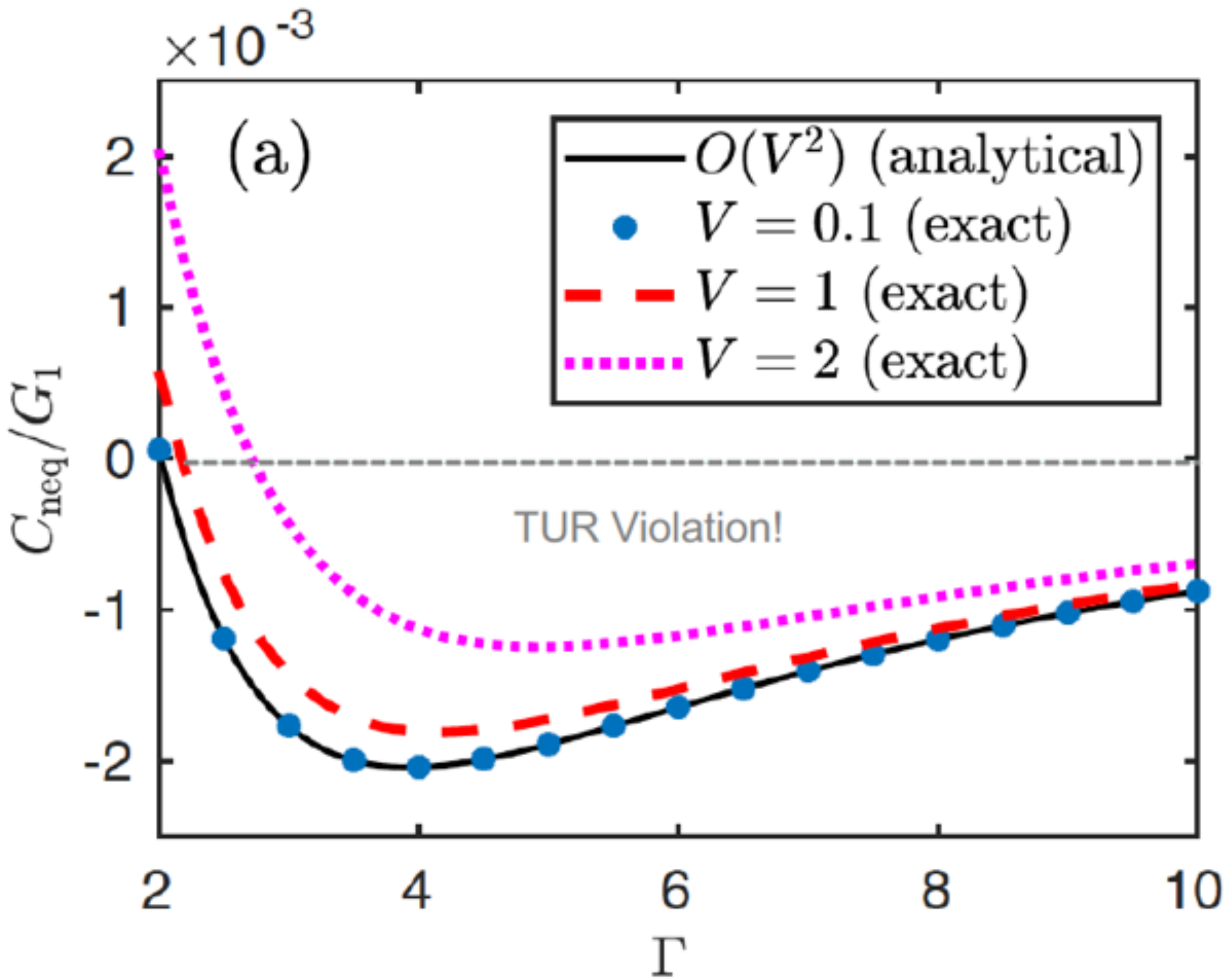
A. single quantum dot B. serial double quantum dot C. side-coupled double quantum dot



Results: Single Quantum Dot

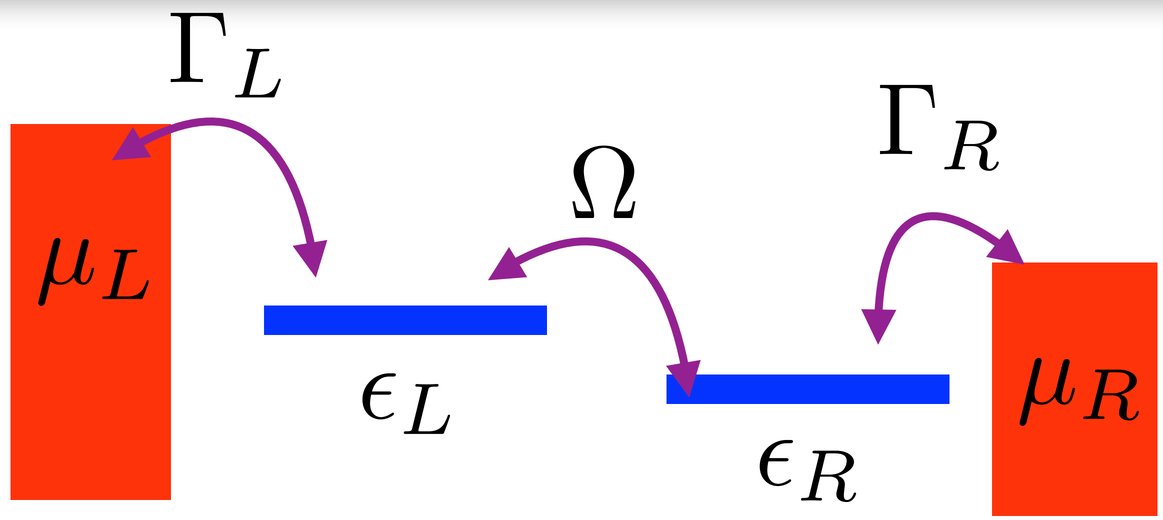


$$\mathcal{T}(E) = \frac{\Gamma_L \Gamma_R}{(E-\epsilon_d)^2 + (\Gamma_L+\Gamma_R)^2/4}$$

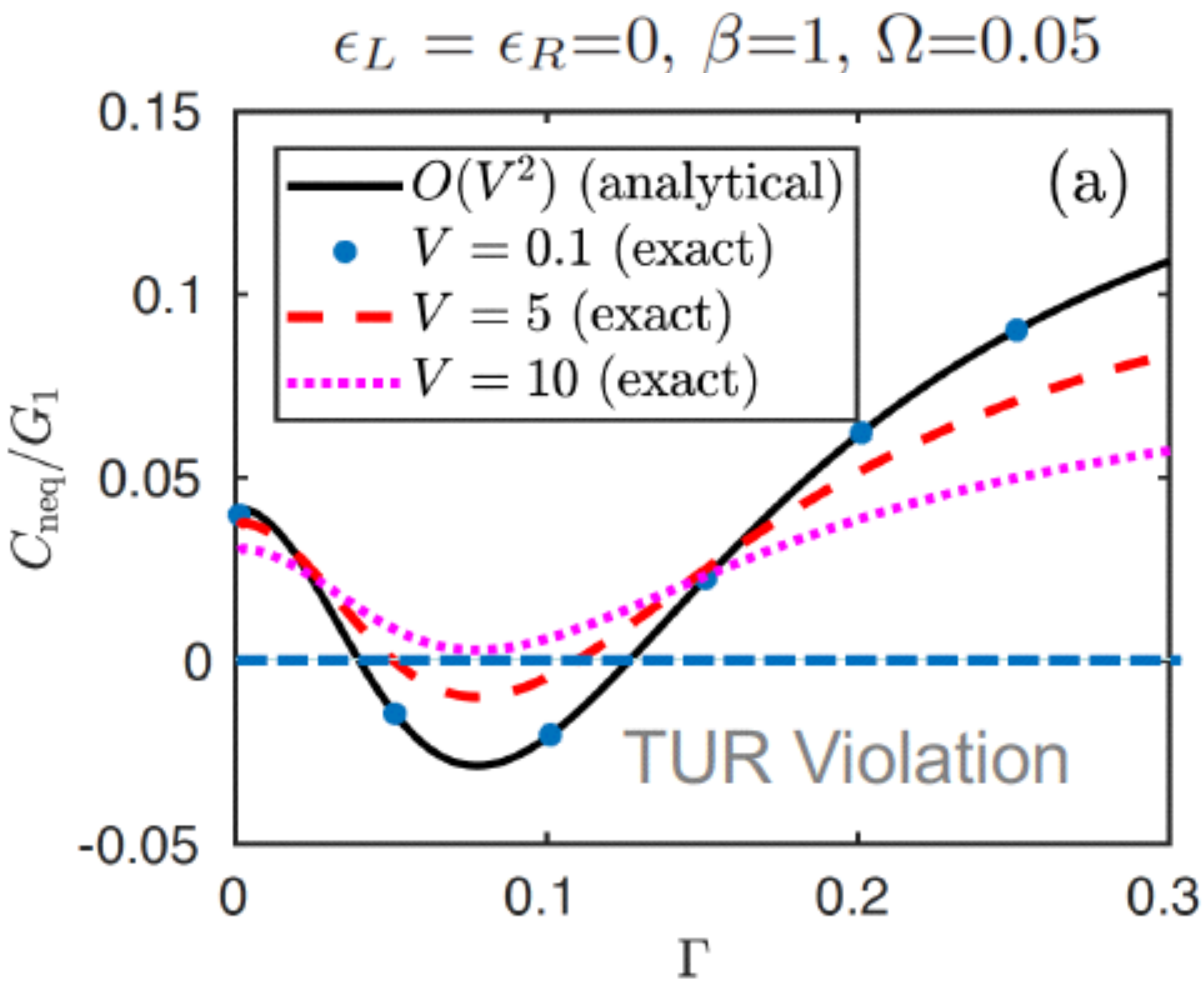


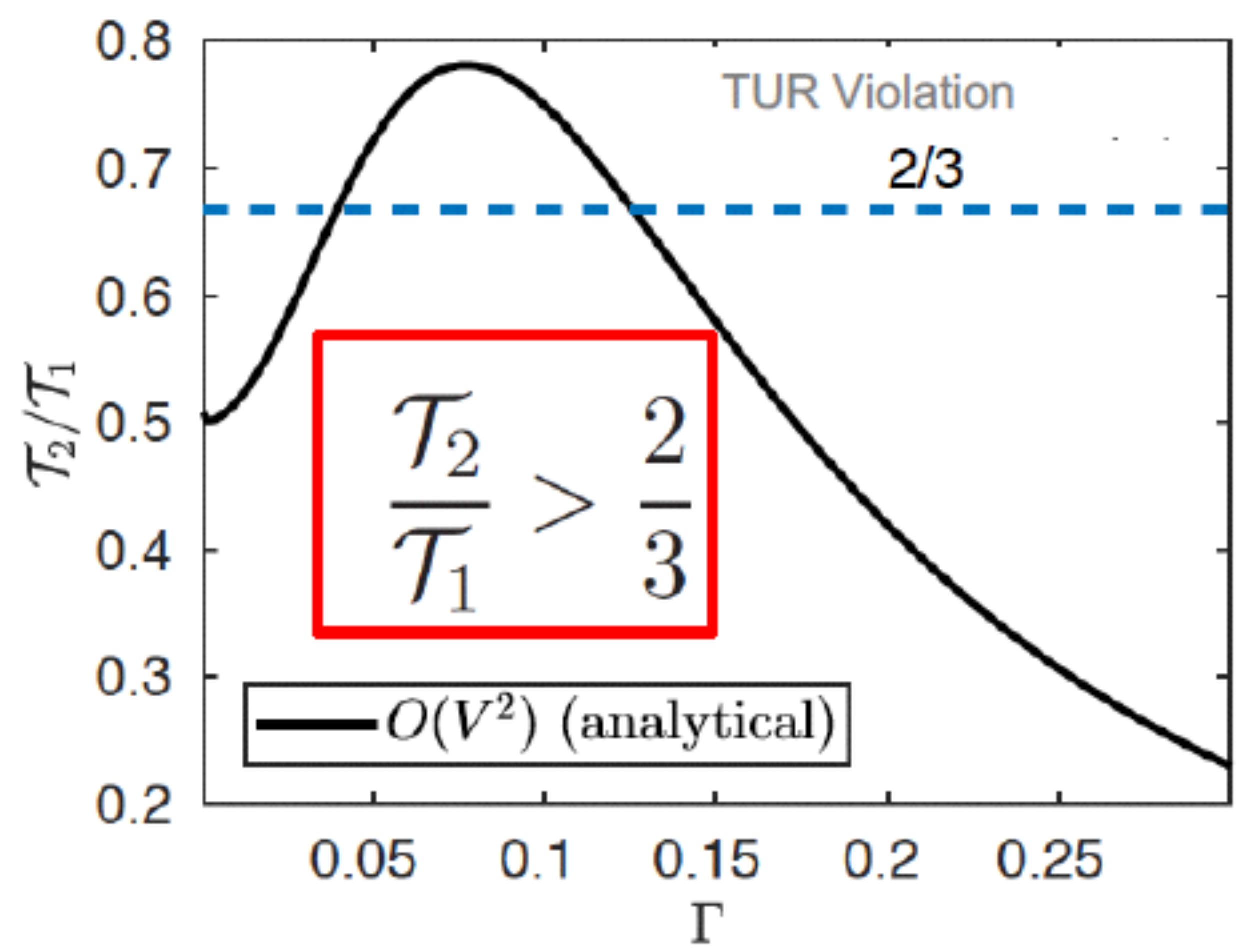
$\epsilon_d = 0, \beta = 1$

Results: Double Quantum Dot



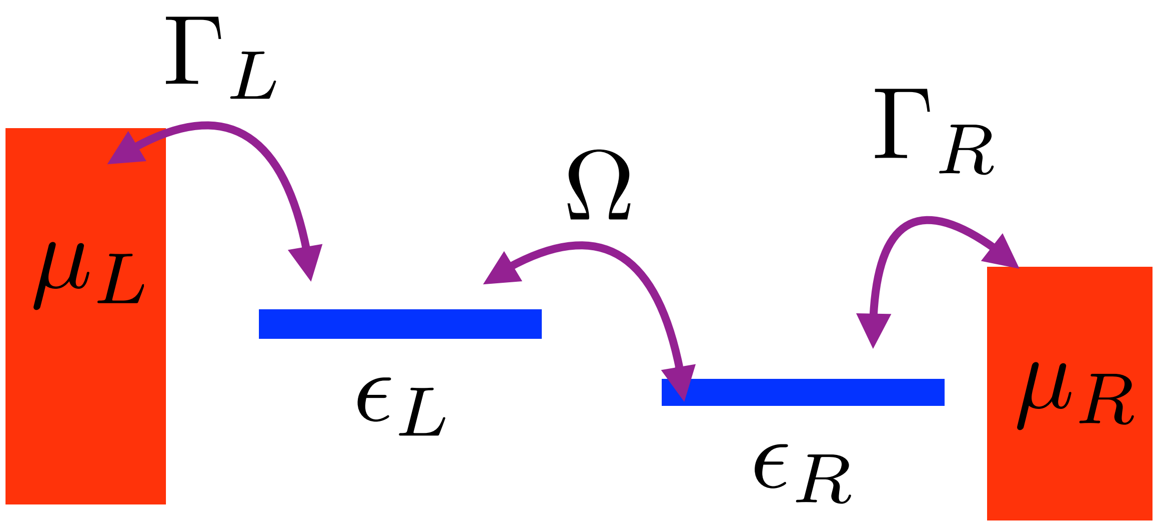
G. Schaller et al PRB (2009)
Harbola et al PRB (2006)

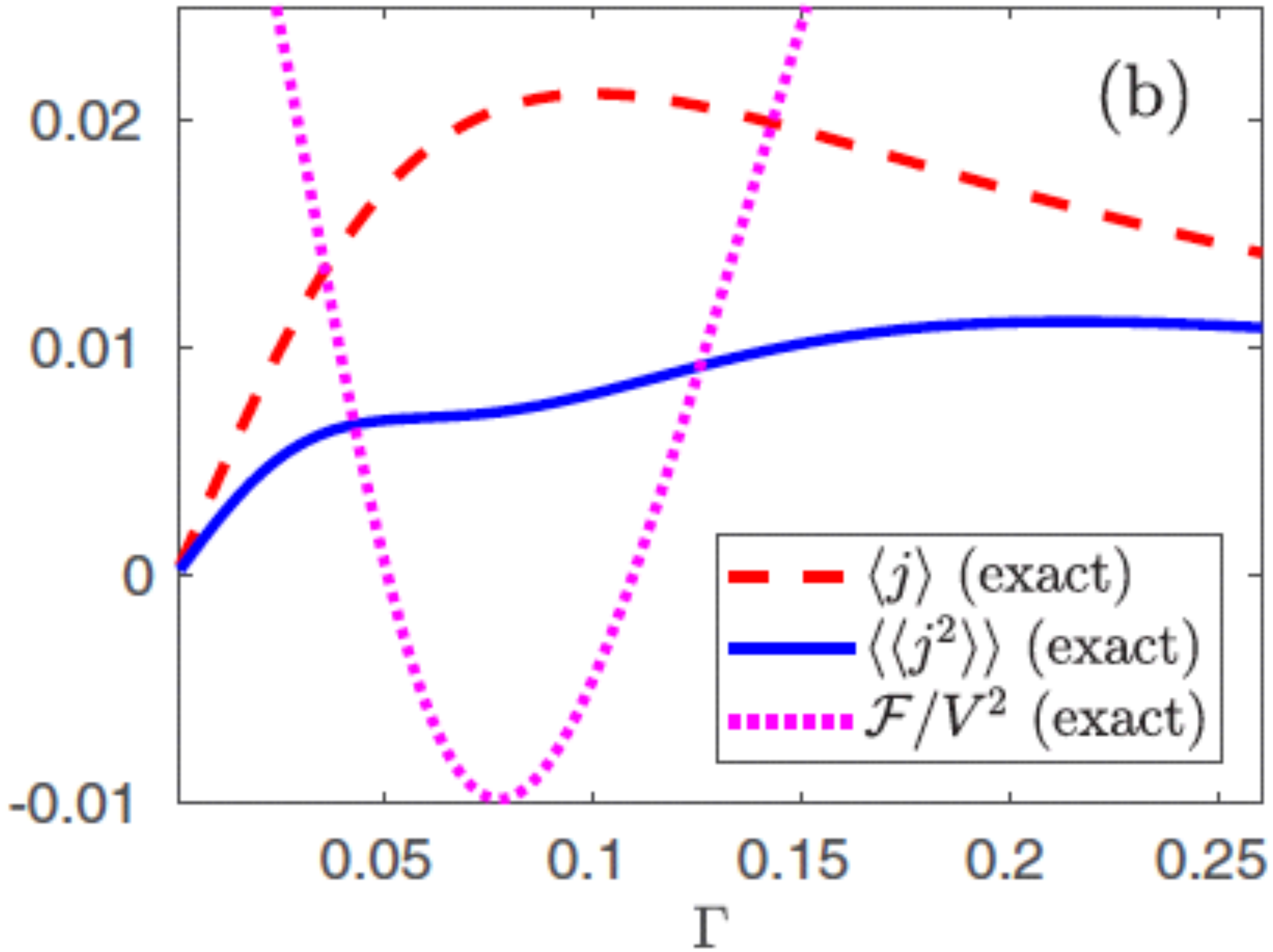




B. K. Agarwalla, D. Segal, PRB (2018)

Results: Double Quantum Dot





TUR: $$\beta V \frac{\langle\langle j^2 \rangle\rangle}{\langle j \rangle} = 2 + \frac{V^2}{G_1} C_{\mathrm{neq}} + \mathcal{O}(V^4) + \cdots$$

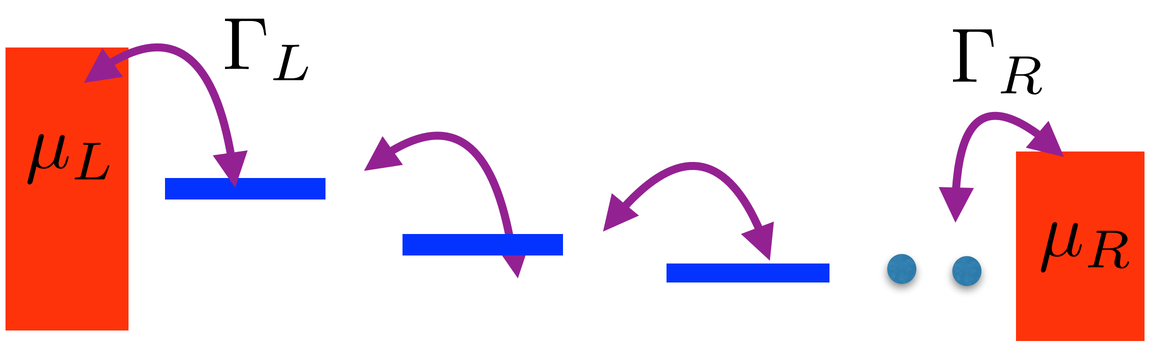
Sign?

$$\frac{\langle\langle j^2 \rangle\rangle}{\langle j \rangle^2} \frac{\sigma}{k_B} \overset{?}{\geq} 2.$$

Table: Thermodynamic uncertainty relation for charge transport in quantum dot setups

hybridization Γ	single dot (A) and side-coupled (C) models	serial double dot model (B)
weak	valid (Markovian master equation for population)	invalid (non-Markovian population dynamics)
strong	invalid (high-order electron tunneling processes)	valid (low transmission function)

Summary:



$$\ln\left[\frac{P_t(+n)}{P_t(-n)}\right] = \beta\,(\mu_L - \mu_R)n$$

$$\frac{\langle\langle j^2\rangle\rangle}{\langle j\rangle^2}\frac{\sigma}{k_B} \overset{?}{\geq} 2.$$

- Thermodynamic uncertainty relation:

  Violation for quantum systems— Depending on the nature of transmission function and external conditions

- What is the bound in the Quantum domain?

Thermodynamics of precision in quantum non equilibrium steady states

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[2]*Instituto de Física da Universidade de São Paulo, 05314-970 São Paulo, Brazil*
[3]*H.H. Wills Physics Laboratory, University of Bristol, Bristol BS8 1TL, UK. and*
[4]*Max Planck Institute for the Structure and Dynamics of Matter, University of Hamburg CFEL, Hamburg, Germany.*
(Dated: February 7, 2019)

Autonomous engines operating at the nano-scale can be prone to deleterious fluctuations in the heat and particle currents which increase, for fixed power output, the more reversible the operation regime is. This fundamental trade-off between current fluctuations and entropy production forms the basis of the recently formulated thermodynamic uncertainty relations (TURs). However, these relations have so far only been derived for classical Markovian systems and can be violated in the quantum regime. In this paper we show that the geometry of quantum non-equilibrium steady-states alone, already directly implies the existence of a TUR, but with a looser bound. The geometrical nature of this result makes it extremely general, establishing a fundamental limit for the thermodynamics of precision. Our proof is based on the McLennan-Zubarev ensemble, which provides an exact description of non-equilibrium steady-states. We first prove that the entropy production of this ensemble can be expressed as a quantum relative entropy. The TURs are then shown to be a direct consequence of the quantum Cramer-Rao bound, a fundamental result from parameter estimation theory. By combining techniques from many-body physics and information sciences, our approach also helps to shed light on the delicate relationship between quantum effects and current fluctuations in autonomous machines, where new general bound on the power output are found and discussed.

$$\frac{\Delta_{\hat{J}_\alpha}}{\langle \hat{J}_\alpha \rangle^2} \langle \hat{\sigma} \rangle \geq \frac{1}{2},$$