Quantum impurities as strongly-coupled open systems

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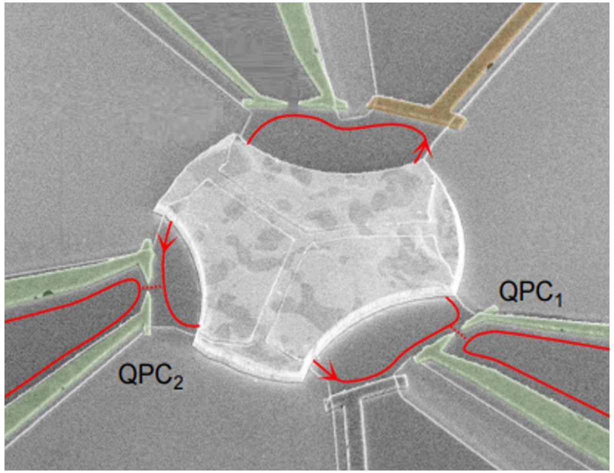

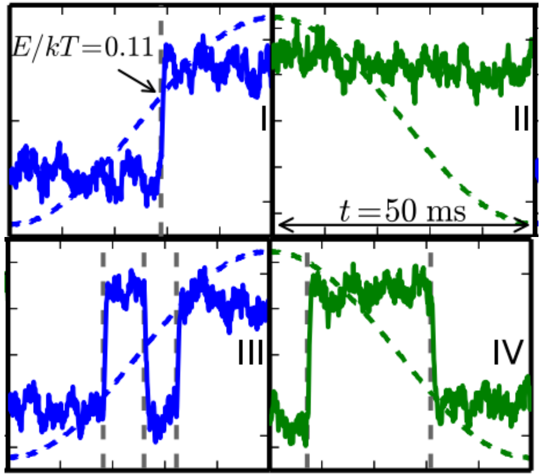

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Outline

Quantum Impurities: perspective on OQS

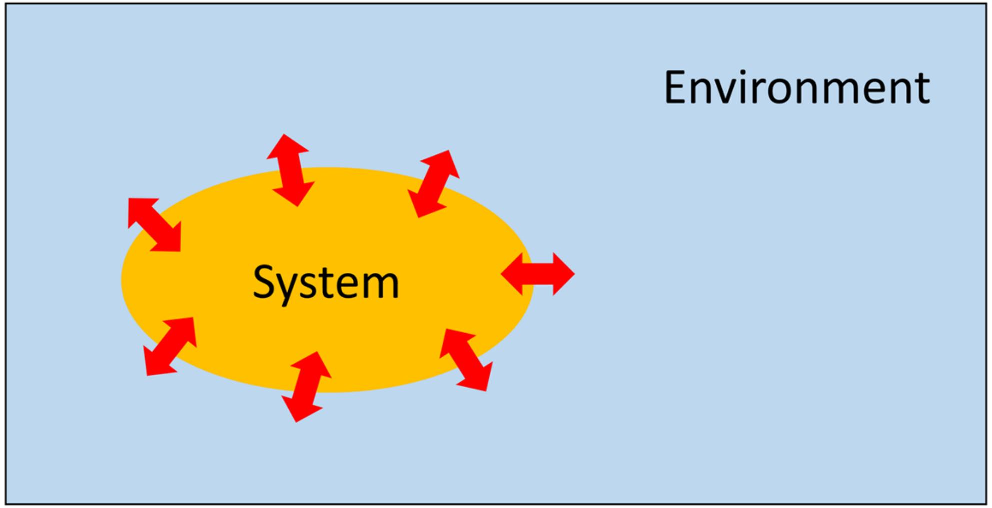
Experimental Platform: quantum dot circuits

Boundary critical phenomena: macroscopic entanglement

External driving: exact dissipated work

Quantum Impurity Models

System and environment treated explicitly



$$H = H_{sys} + H_{env} + H_{hyb}$$

Bath in thermodynamic limit (typically non-interacting)

$$J(\omega) = \pi \sum_k |\gamma_k|^2 \, \delta(\omega - \epsilon_k)$$

Spin-boson model:

$$H_{\mathrm{SB}} = \underbrace{\left(-\frac{\Delta}{2}\sigma_x + \frac{\epsilon}{2}\sigma_z\right)}_{H_{\mathrm{sys}}} + \underbrace{\sum_k \omega_k \, b_k^\dagger b_k}_{H_{\mathrm{env}}} + \underbrace{\frac{\sigma_z}{2}\sum_k \lambda_k \left(b_k^\dagger + b_k\right)}_{H_{\mathrm{hyb}}}$$

Leggett et al., RMP 59, 1 (1987)

Quantum Impurity Models

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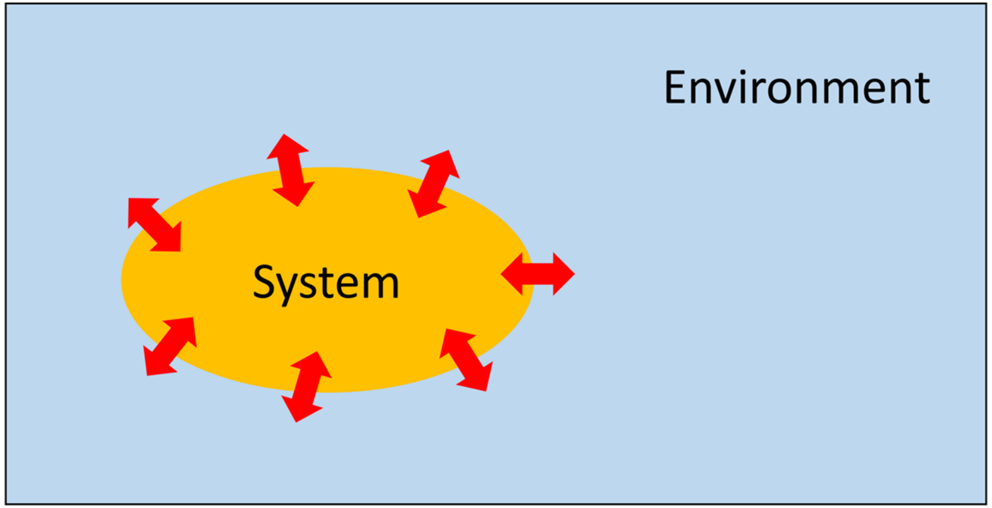

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Kondo model:

$$H_{\mathrm{K}} = \underbrace{\left(-h S^z_{\mathrm{imp}}\right)}_{H_{\mathrm{sys}}} + \underbrace{\sum_{k\sigma} \epsilon_k \, c^\dagger_{k\sigma} c_{k\sigma}}_{H_{\mathrm{env}}} + \underbrace{J \, \mathbf{S}_{\mathrm{imp}} \cdot \sum_{kk'} \sum_{\alpha\beta}}_{H_{\mathrm{hyb}}} \gamma_k \gamma^*_{k'} c^\dagger_{k\alpha} \frac{\boldsymbol{\sigma}_{\alpha\beta}}{2} c_{k'\beta}$$

Hewson, *"Kondo problem to Heavy fermions"* CUP (1995)

Open Quantum System picture

Want an approximate equation of motion for: $\rho_{\text{sys}}(t) = \text{Tr}_{\text{env}}\, \rho_{\text{tot}}(t)$

Born approximation: assume weak system-bath coupling such that

$\rho_{\text{tot}}(t) \approx \rho_{\text{sys}}(t) \otimes \rho_{\text{env}}$ with a stationary bath $[H_{\text{env}}, \rho_{\text{env}}] = 0$

Neglect persistent system-bath correlations beyond 2nd order in H_{hyb}

Markov approximation: neglect memory effects, assuming short environmental correlation times, $\tau_{\text{env}} \ll \tau_{\text{sys}}$

Redfield equation (interaction picture):

$$\frac{d\tilde{\rho}_{\text{sys}}(t)}{dt} = -\int_0^\infty d\tau\; \text{Tr}_{\text{env}} \left[\widetilde{H}_{\text{hyb}}(t), \left[\widetilde{H}_{\text{hyb}}(t-\tau), \tilde{\rho}_{\text{sys}}(t) \otimes \rho_{\text{env}} \right] \right]$$

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Further secular approximation → GKSL/Lindblad

$$\dot{\rho}_{\text{sys}} = -i\left[H_{\text{eff}}, \rho_{\text{sys}}\right] + \sum_j \left(L_j \rho_{\text{sys}} L_j^\dagger - \frac{1}{2}\left\{ L_j^\dagger L_j, \rho_{\text{sys}} \right\} \right)$$

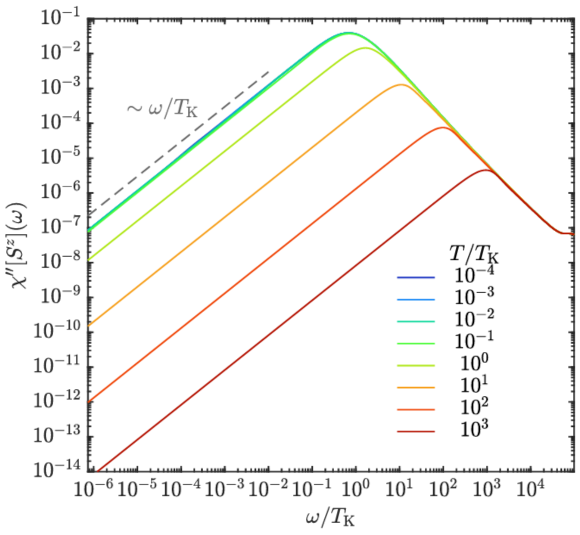
Quantum Impurity Models

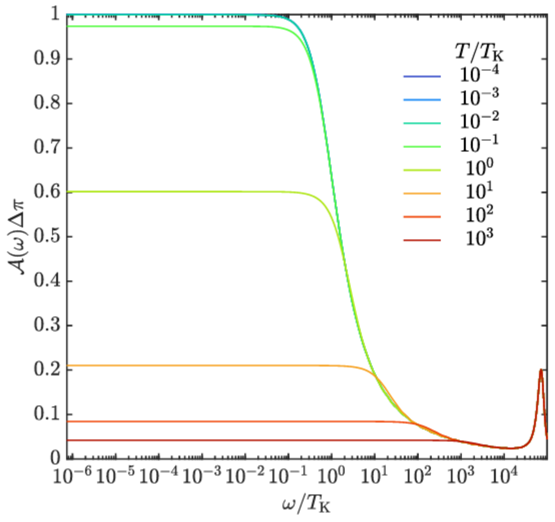
Strong coupling limit: System and bath are entangled and can become strongly correlated. Dynamics are non-Markovian.

→ Many-body system

→ Non-trivial retarded correlation functions

→ E.g. boundary criticality





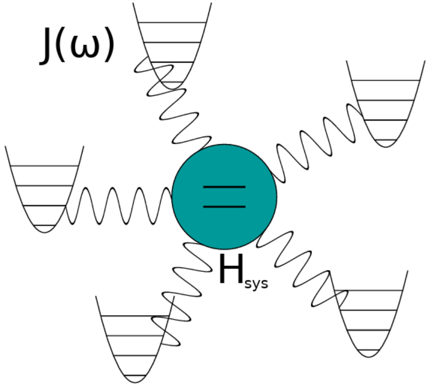
First we take system-bath composite system at thermal equilibrium

→ later we'll consider external driving from this initial state

Example: spin-boson model

Particle in double-well potential coupled to dissipative environment

$$H_{\mathrm{SB}} = \underbrace{\left(-\frac{\Delta}{2}\sigma_x + \frac{\epsilon}{2}\sigma_z\right)}_{H_{\mathrm{sys}}} + \underbrace{\sum_k \omega_k\, b_k^\dagger b_k}_{H_{\mathrm{env}}} + \underbrace{\frac{\sigma_z}{2}\sum_k \lambda_k \left(b_k^\dagger + b_k\right)}_{H_{\mathrm{hyb}}}$$



Dissipative localization transition:

→ inherently a non-perturbative many-body bath effect (not captured by weak-coupling Markovian master equation)

→ Non-local-in-time influence functional

→ Kosterlitz–Thouless transition separating delocalized & localized phases

→ Spin flip displaces low-frequency oscillators: orthogonality catastrophe

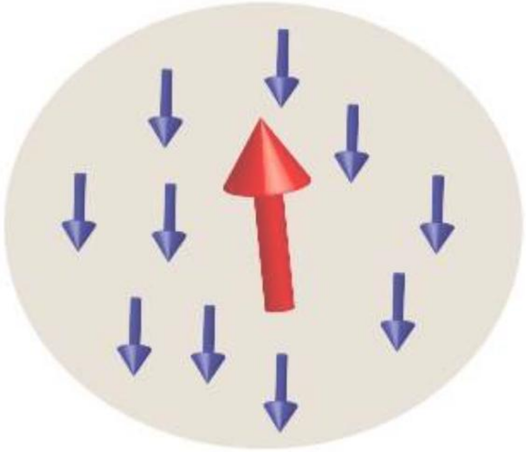
→ Non-perturbative renormalized tunneling rates

Leggett et al., Rev. Mod. Phys. 59, 1 (1987)

Example: Kondo model

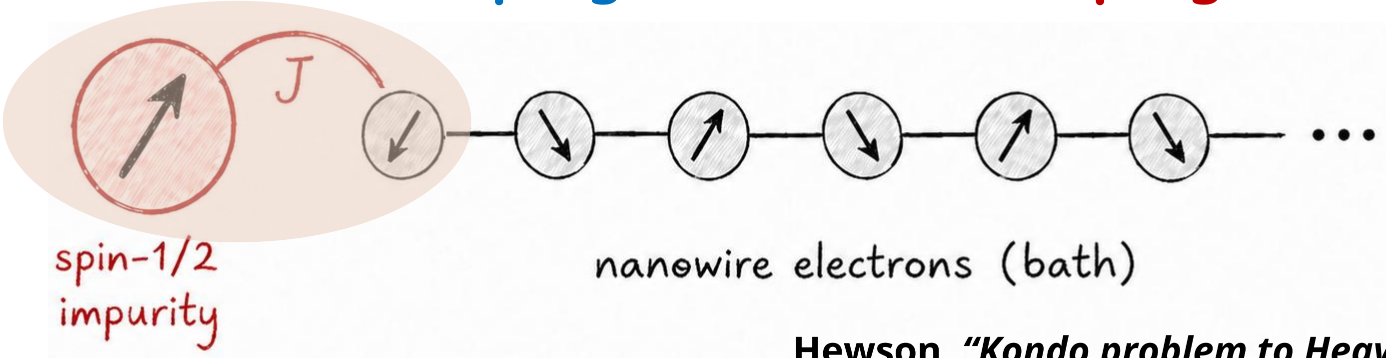
Magnetic impurity coupled to conduction electrons

$$H_{\mathrm{K}} = \underbrace{\left(-hS^z_{\mathrm{imp}}\right)}_{H_{\mathrm{sys}}} + \underbrace{\sum_{k\sigma} \epsilon_k \, c^\dagger_{k\sigma} c_{k\sigma}}_{H_{\mathrm{env}}} + \underbrace{J\, \mathbf{S}_{\mathrm{imp}} \cdot \mathbf{S}_{\mathrm{env}}}_{H_{\mathrm{hyb}}}$$



Impurity spin screened by surrounding electronic "entanglement cloud"

→ **Renormalized couplings: No weak-coupling limit!**



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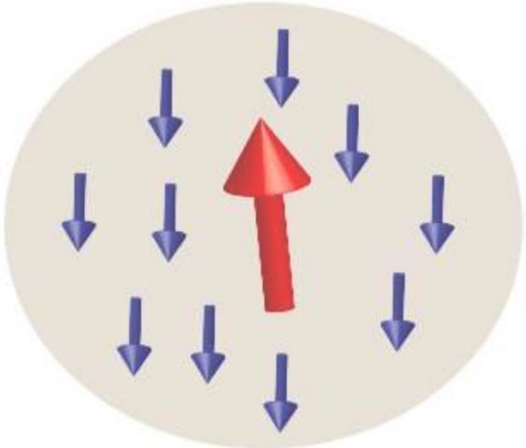

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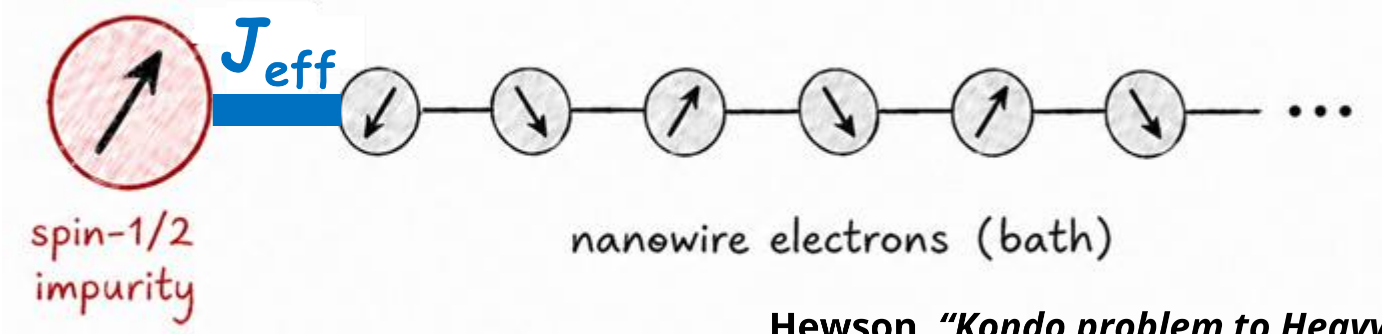

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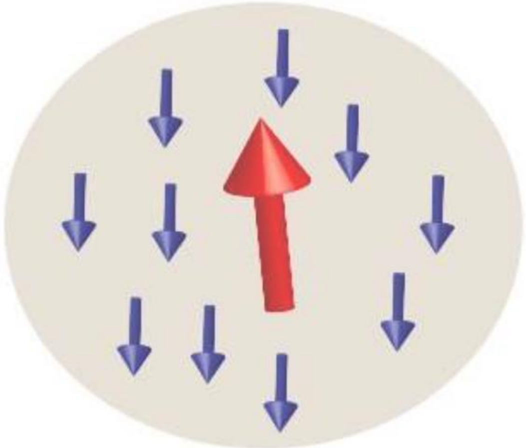

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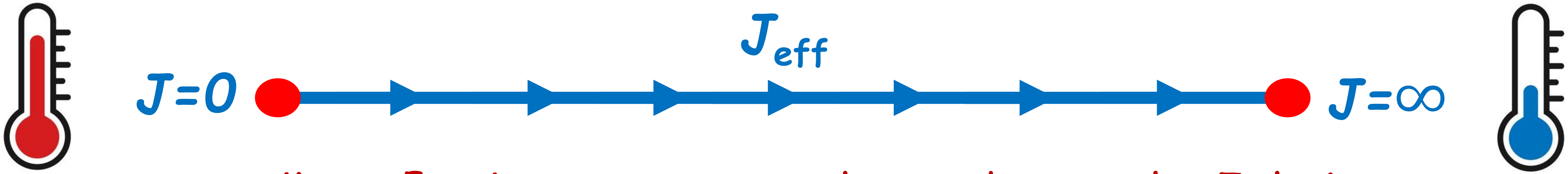


… so no Master Equation can ever capture the ground state or low-T physics …

Local description

Can we approximate dissipation into bath using an effective local model?

$$H_{\mathrm{RLM}} = \underbrace{\epsilon_d\, d^\dagger d}_{H_{\mathrm{sys}}} + \underbrace{\sum_k \epsilon_k\, c_k^\dagger c_k}_{H_{\mathrm{env}}} + \underbrace{\sum_k \left(V_k d^\dagger c_k + V_k^* c_k^\dagger d \right)}_{H_{\mathrm{hyb}}}$$

Spinless, non-interacting resonant level model

Exact impurity RDM: $$\rho_{\mathrm{imp}} = \begin{pmatrix} 1 - n_d & 0 \\ 0 & n_d \end{pmatrix} = \frac{e^{-\beta H^*_{\mathrm{imp}}}}{Z^*_{\mathrm{imp}}}$$

Hamiltonian of mean force

$$H^*_{\mathrm{imp}} = \epsilon^*_d(T)\, d^\dagger d$$

$$n_d = f(\epsilon^*_d)$$

Exactly reproduces local static quantities…

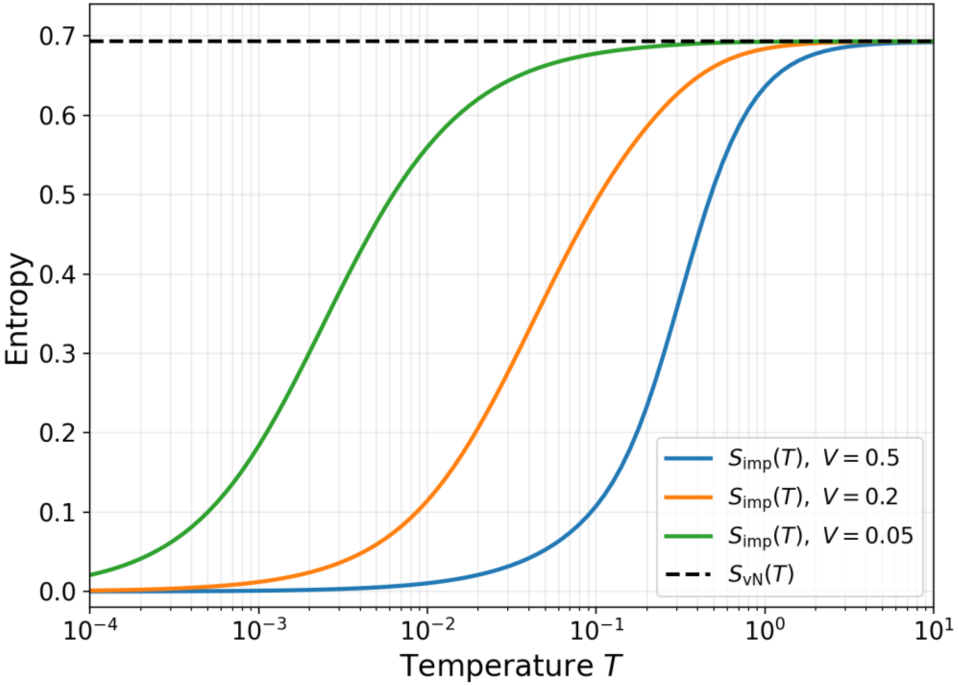
$$\Rightarrow \quad \epsilon^*_d(T) = T \ln\left(\frac{1 - n_d}{n_d}\right)$$

Impurity entropy

Von Neumann entropy of impurity reduced state: $S_{\mathrm{vN}} = -\operatorname{Tr} \rho_{\mathrm{imp}} \ln \rho_{\mathrm{imp}}$

Wilson impurity contribution to total entropy: $S_{\mathrm{imp}}(T) = S_{\mathrm{tot}}(T) - S^{(0)}_{\mathrm{env}}(T)$

Example: half-filling
($n_d=1/2 \rightarrow S_{vN}=\ln 2$)

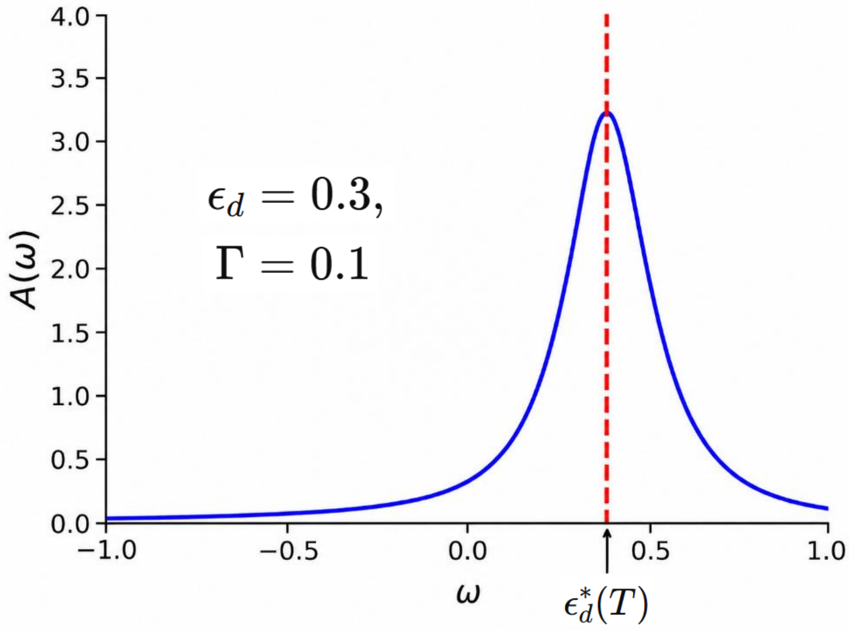


S_{vN} does not reflect total entropy changes due to system-bath correlations

Local dynamics

Impurity Green's function from Hamiltonian of mean force: $G^R_{\mathrm{HMF}}(\omega) = \dfrac{1}{\omega - \epsilon_d^*(T) + i0^+}$

Impurity spectral function: $A_{\mathrm{HMF}}(\omega) = -\dfrac{1}{\pi}\,\mathrm{Im}\,G^R_{\mathrm{HMF}}(\omega) = \delta(\omega - \epsilon_d^*(T))$



True impurity Green's function (wide-flat-band limit):

$$G^R_d(\omega) = \frac{1}{\omega - \epsilon_d + i\Gamma}$$

Effective non-Hermitian model:

$$H_{\mathrm{NH}} = \epsilon^*\, d^\dagger d \qquad \epsilon^* = \epsilon_d - i\Gamma$$

(can also incorporate Lamb shift)

Problem of interactions

Does not straightforwardly generalize to many-body problems with interactions

Simplest example: Anderson model

$$H_{\text{AIM}} = \underbrace{\sum_{\sigma} \epsilon_d \, n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow}}_{H_{\text{sys}}} + \underbrace{\sum_{k\sigma} \epsilon_k \, c^{\dagger}_{k\sigma} c_{k\sigma}}_{H_{\text{env}}} + \underbrace{\sum_{k\sigma} \left(V_k d^{\dagger}_{\sigma} c_{k\sigma} + V^{*}_{k} c^{\dagger}_{k\sigma} d_{\sigma} \right)}_{H_{\text{hyb}}}$$

Exact impurity RDM: $\rho_{\text{imp}} = \begin{pmatrix} p_0 & 0 & 0 & 0 \\ 0 & p_\uparrow & 0 & 0 \\ 0 & 0 & p_\downarrow & 0 \\ 0 & 0 & 0 & p_2 \end{pmatrix}$

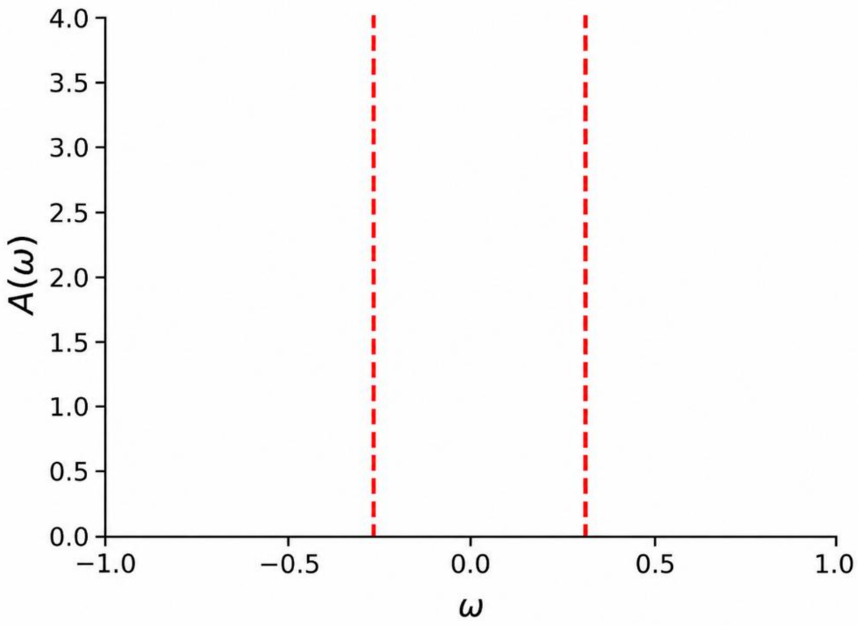
$$\left.\begin{aligned} p_\uparrow &= p_\downarrow = \frac{n_d}{2} - D, \\ p_2 &= D, \\ p_0 &= 1 - n_d + D \end{aligned}\right\} \quad \begin{aligned} \frac{n_d}{2} &= \langle n_{d\uparrow} \rangle = \langle n_{d\downarrow} \rangle \\ D &= \langle n_{d\uparrow} n_{d\downarrow} \rangle \end{aligned}$$

Corresponding HMF: $H^{*}_{\text{imp}} = \epsilon^{*}_{d} \sum_{\sigma} n_{d\sigma} + U^{*} n_{d\uparrow} n_{d\downarrow}$ $\quad \epsilon^{*}_{d} = T \ln \left(\frac{1 - n_d + D}{\frac{n_d}{2} - D} \right)$ $\quad U^{*} = T \ln \left[\frac{\left(\frac{n_d}{2} - D\right)^2}{D(1 - n_d + D)} \right]$

Problem of interactions

Green's function from Hamiltonian of mean force: $$G^R_{\mathrm{HMF}}(\omega, T) = \frac{1}{\omega + i0^+ - \epsilon_d^*(T) - \Sigma_d^*(\omega, T)}$$

True impurity Green's function (wide-flat-band limit): $$G^R_d(\omega, T) = \frac{1}{\omega + i0^+ - \epsilon_d + i\Gamma - \Sigma_d^R(\omega, T)}$$



HMF does not capture environmental lifetime broadening effects!

Problem of interactions

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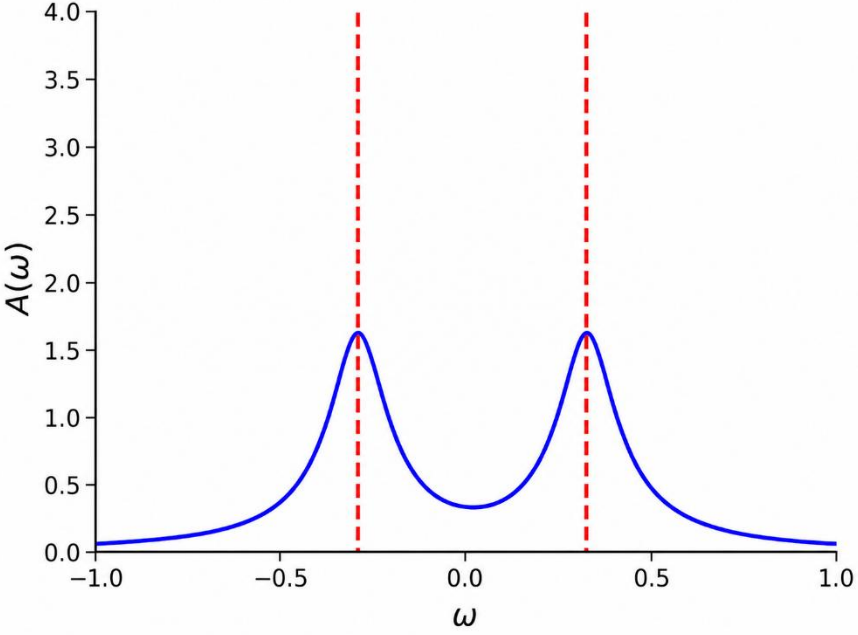


Can we just use the isolated system self-energy with the bath hybridization? ("Hubbard-I")

Equivalent to non-Hermitian local Hamiltonian:

$$H_{\mathrm{NH}} = \sum_\sigma \epsilon_d^* n_{d\sigma} + U\, n_{d\uparrow} n_{d\downarrow}$$

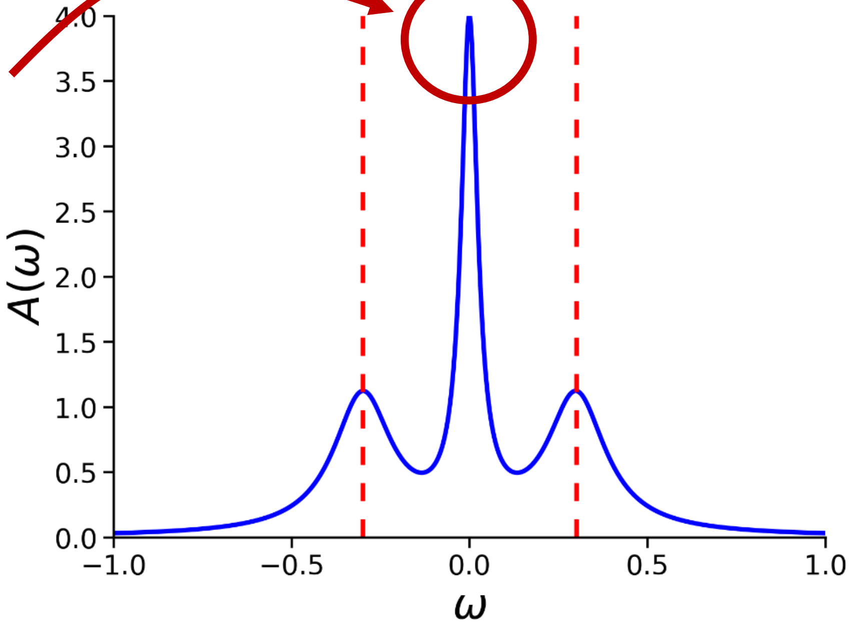
with $\epsilon_d^* = \epsilon_d - i\Gamma$

Problem of interactions

Green's function from Hamiltonian of mean force: $$G^R_{\mathrm{HMF}}(\omega,T)=\frac{1}{\omega+i0^+-\epsilon^*_d(T)-\Sigma^*_d(\omega,T)}$$

True impurity Green's function (wide-flat-band limit): $$G^R_d(\omega,T)=\frac{1}{\omega+i0^+-\epsilon_d+i\Gamma-\Sigma^R_d(\omega,T)}$$

system-bath coherence peak



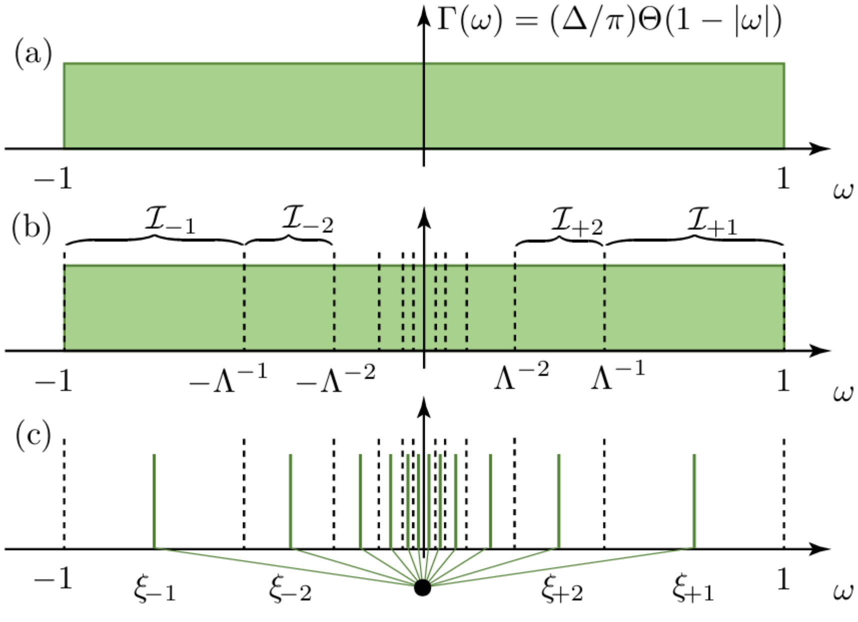
True self-energy must be computed in the presence of the bath

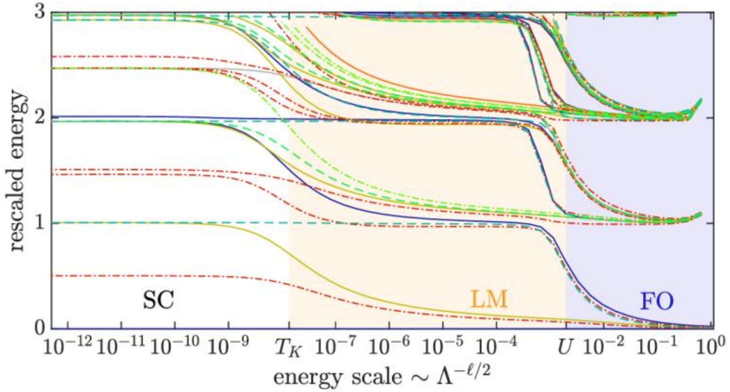
No local HMF or NH Hamiltonian can capture the many-body physics

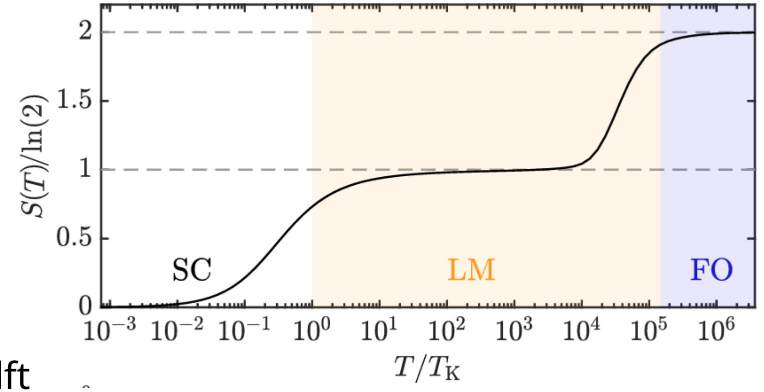
→ Kondo effect!

Numerical Renormalization Group

In equilibrium, with a non-interacting bath, quantum impurity models can be solved numerically-exactly using Wilson's NRG







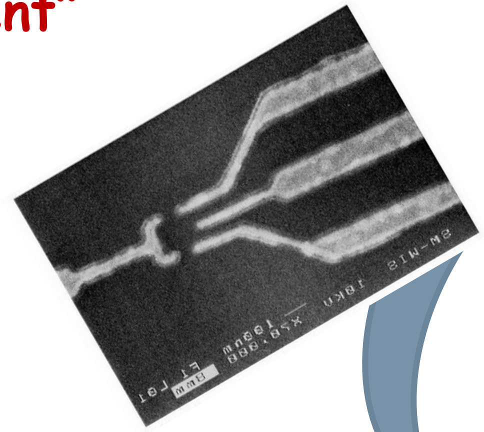
see Bulla et al., Rev. Mod. Phys. 80, 395 (2008); figures courtesy of J von Delft

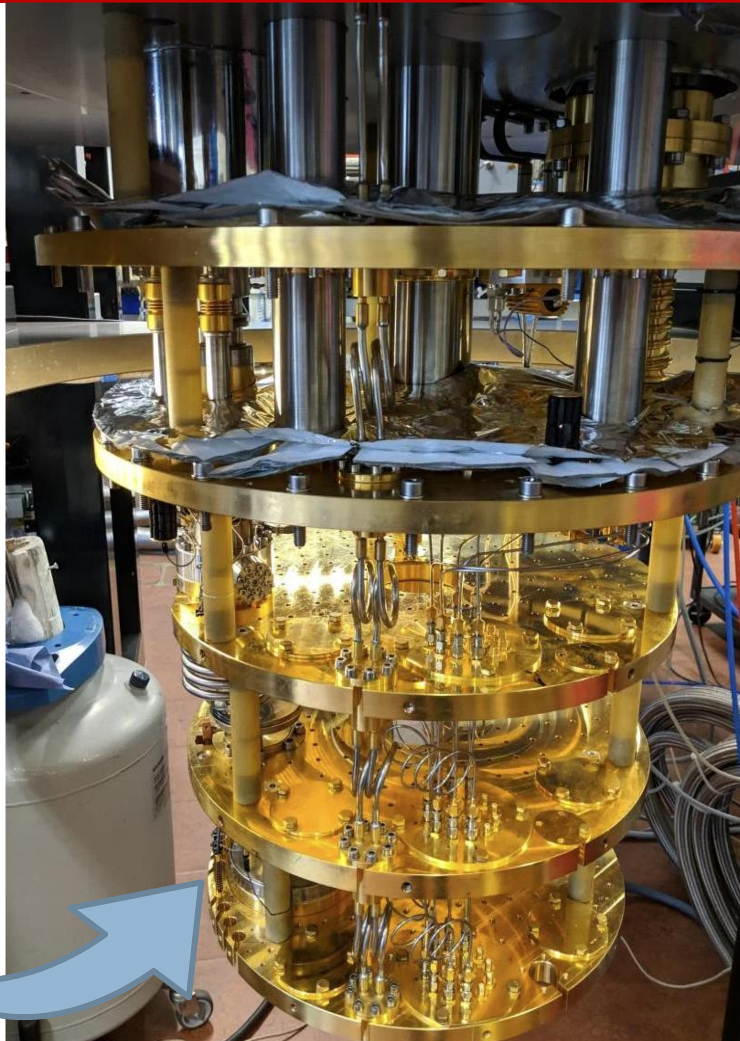
Quantum dot devices

Nanoelectronic circuit:

- Open quantum system
- Nanostructure: “system”
- Leads: fermionic “environment”

- Strong coupling
- Many-body physics
- Strongly non-Markovian





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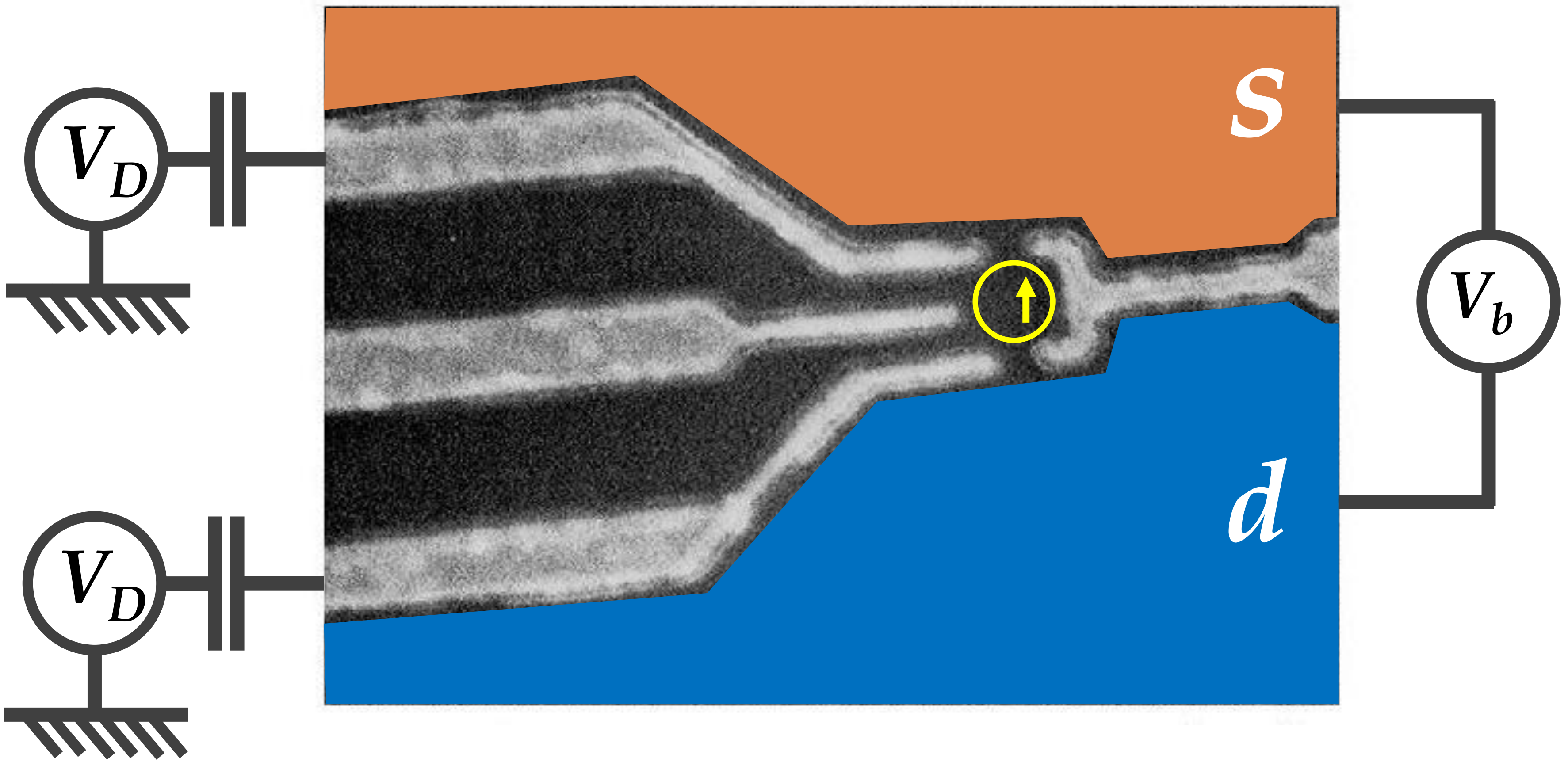
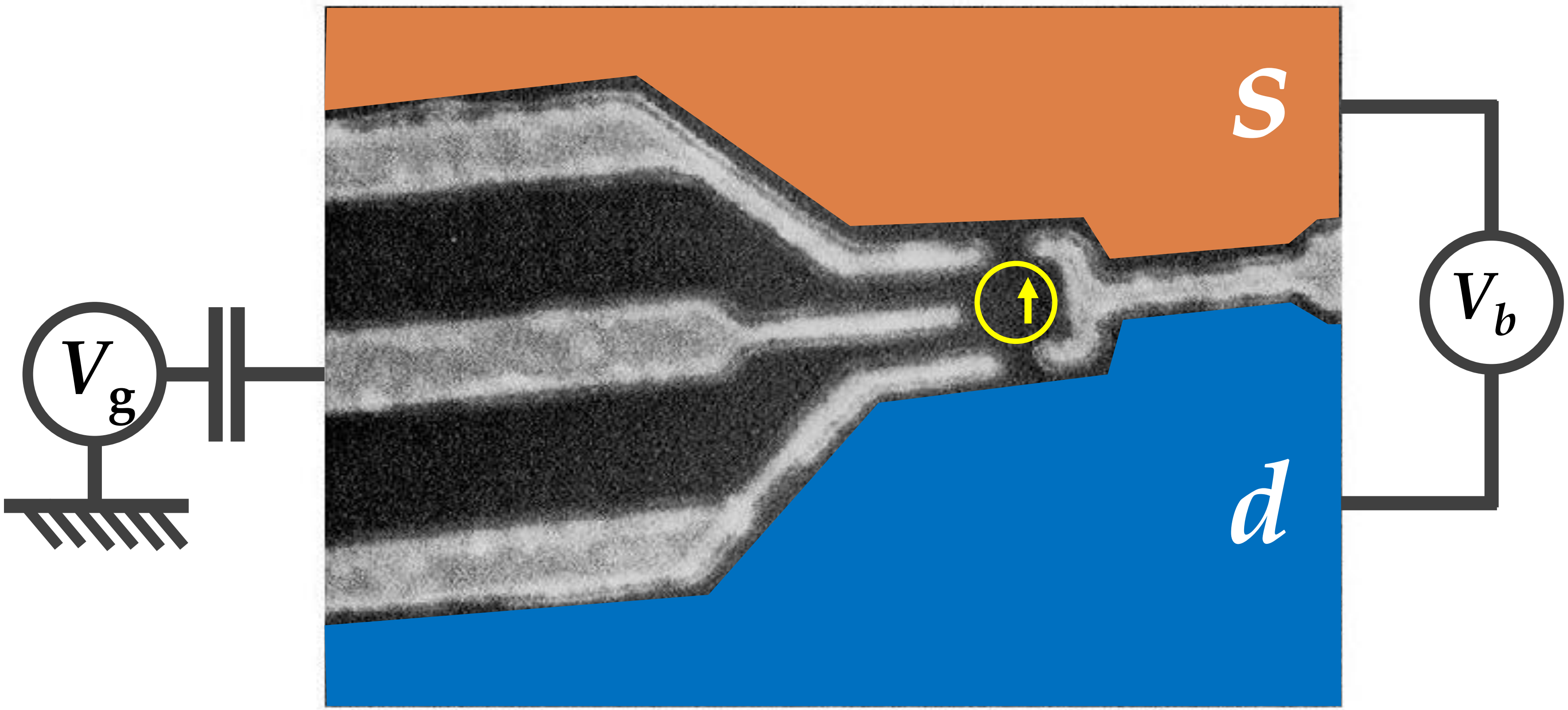


Goldhaber-Gordon *et al.*, Nature 391, 156 (1998)

Quantum dot devices



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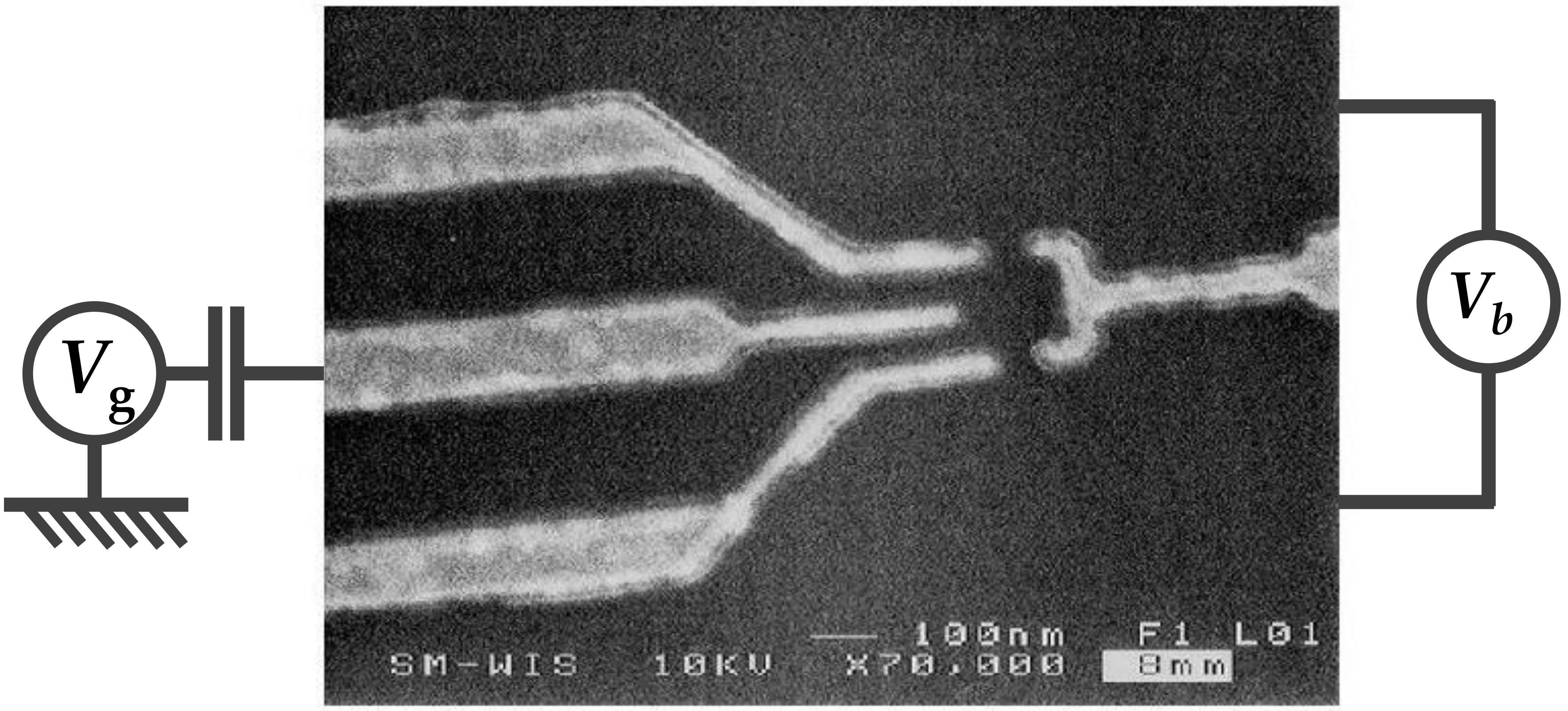
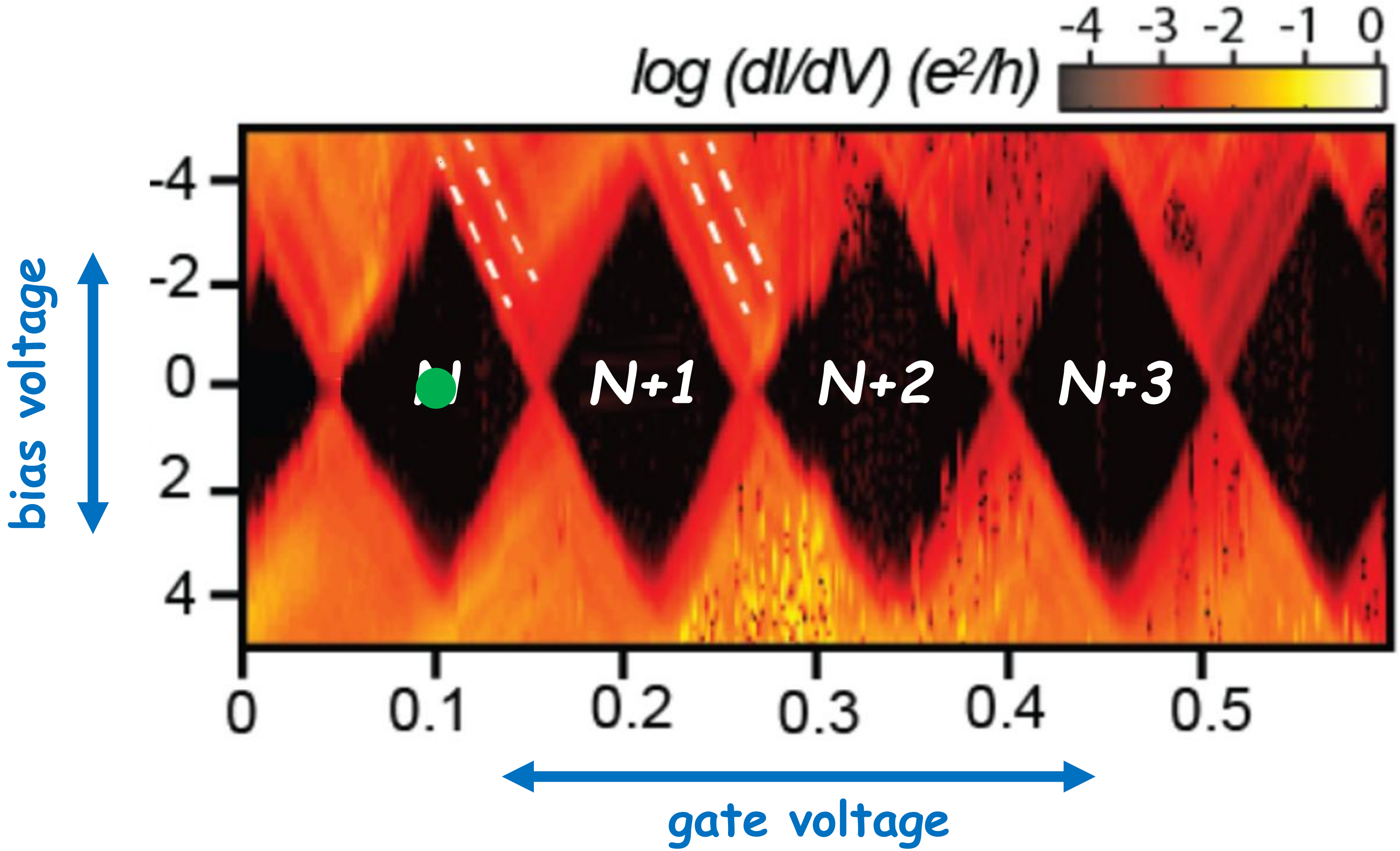
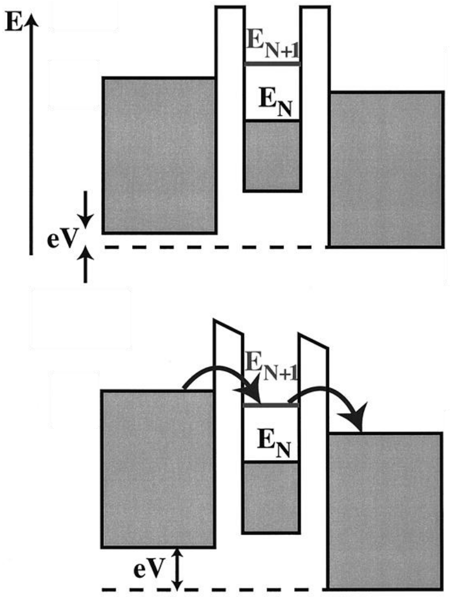


Goldhaber-Gordon *et al.*, Nature 391, 156 (1998)

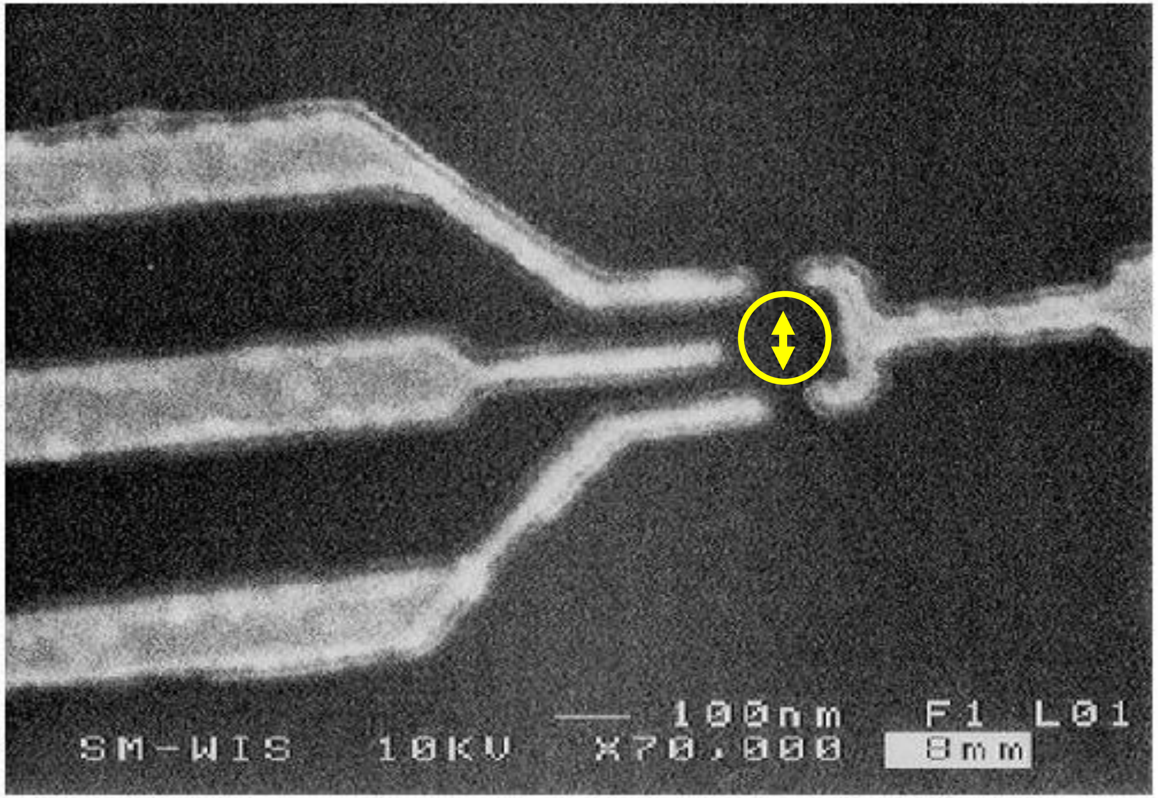
Strong correlations: Coulomb blockade





Ganjipour *et al*, PRB 91, 161301 (2015)

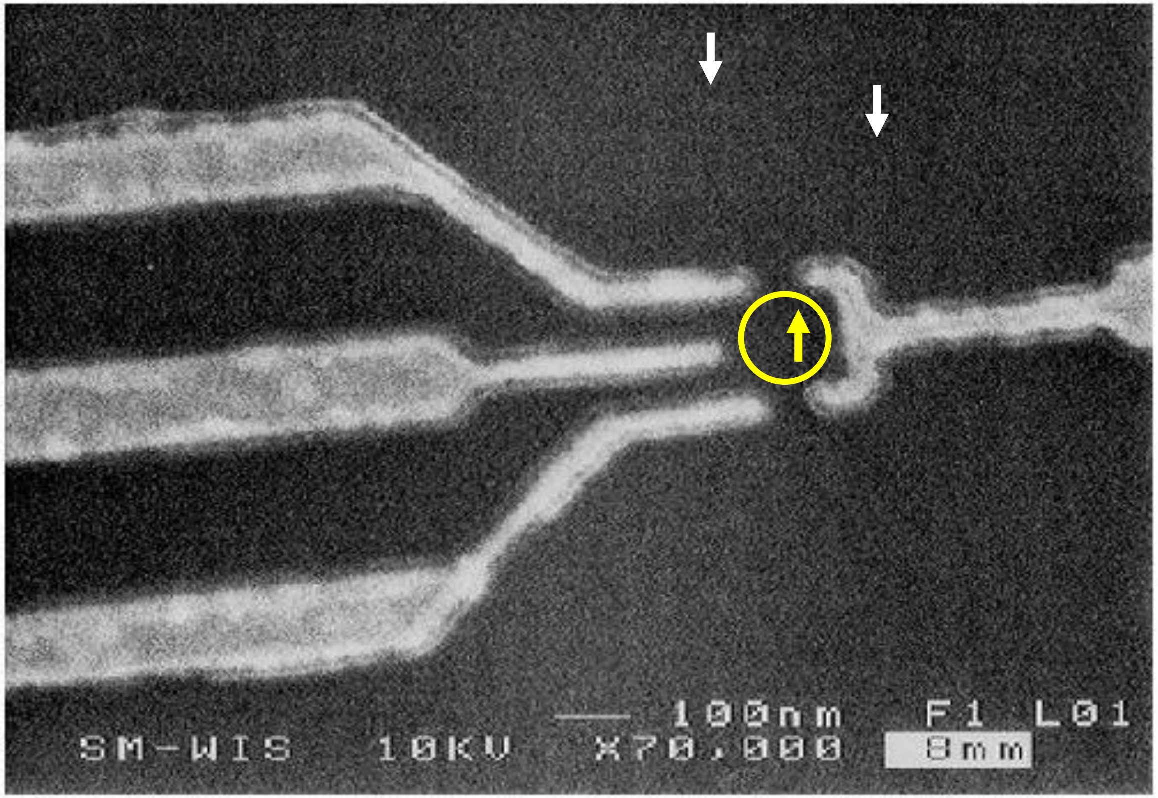
Trapped spin-1/2 qubit



PW Anderson, "*Localized magnetic states in metals*" Physical Review 124, 41 (1961)

Trapped spin-1/2 qubit

QD can be regarded as an open quantum system



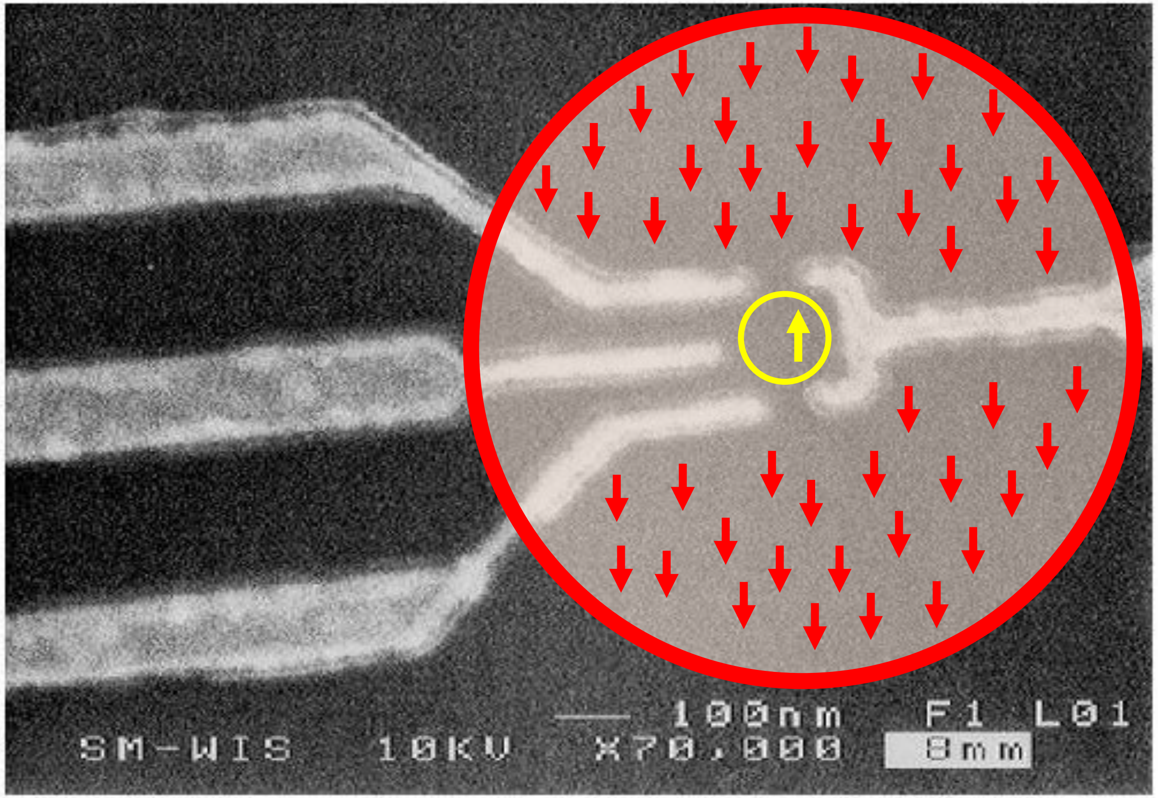
qubit is strongly coupled to the fermionic bath

non-Markovian

PW Anderson, "*Localized magnetic states in metals*" Physical Review 124, 41 (1961)

QD-lead entanglement: Kondo effect

QD can be regarded as an open quantum system

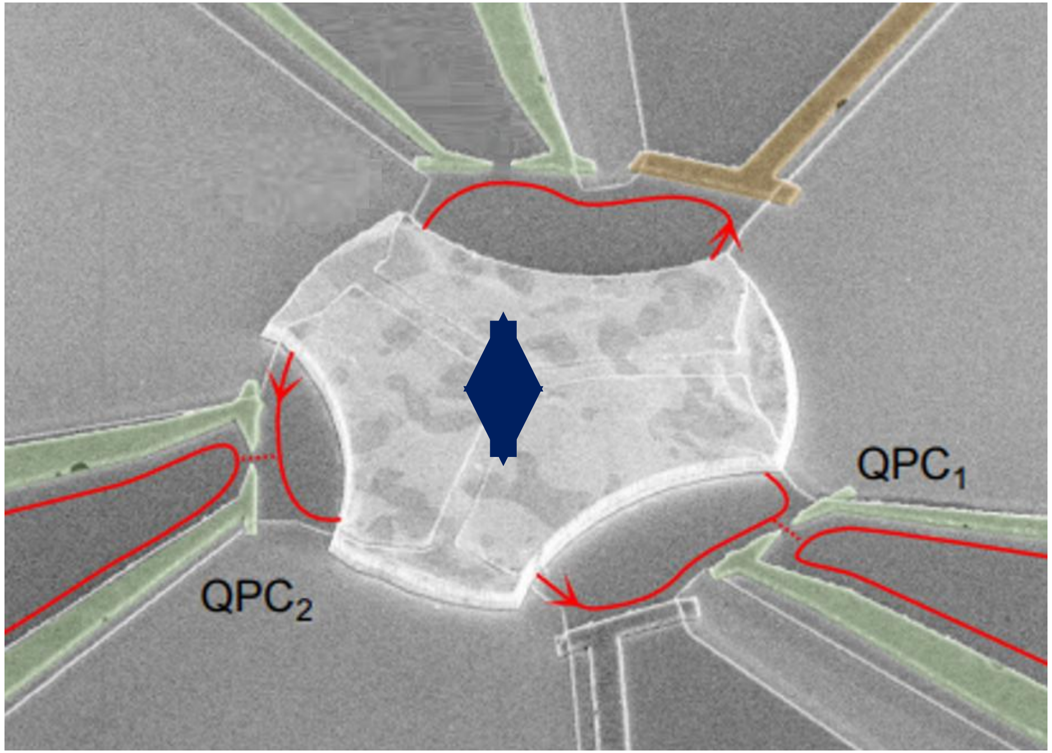


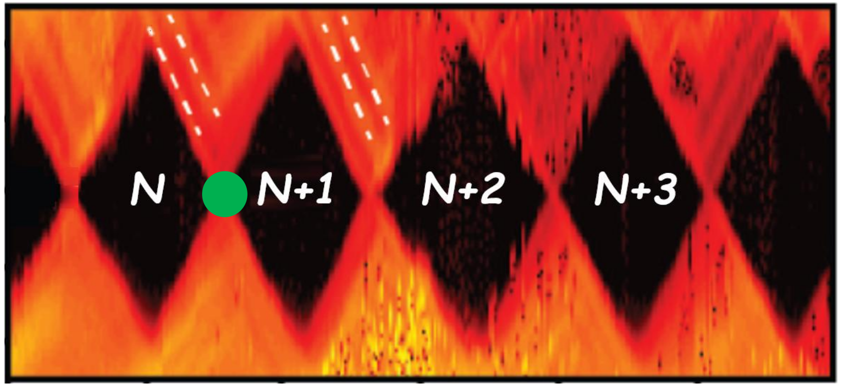
qubit is strongly coupled to the fermionic bath

non-Markovian

AC Hewson, "*The Kondo effect to Heavy Fermions*", CUP 1999

Large QDs: charge qubit



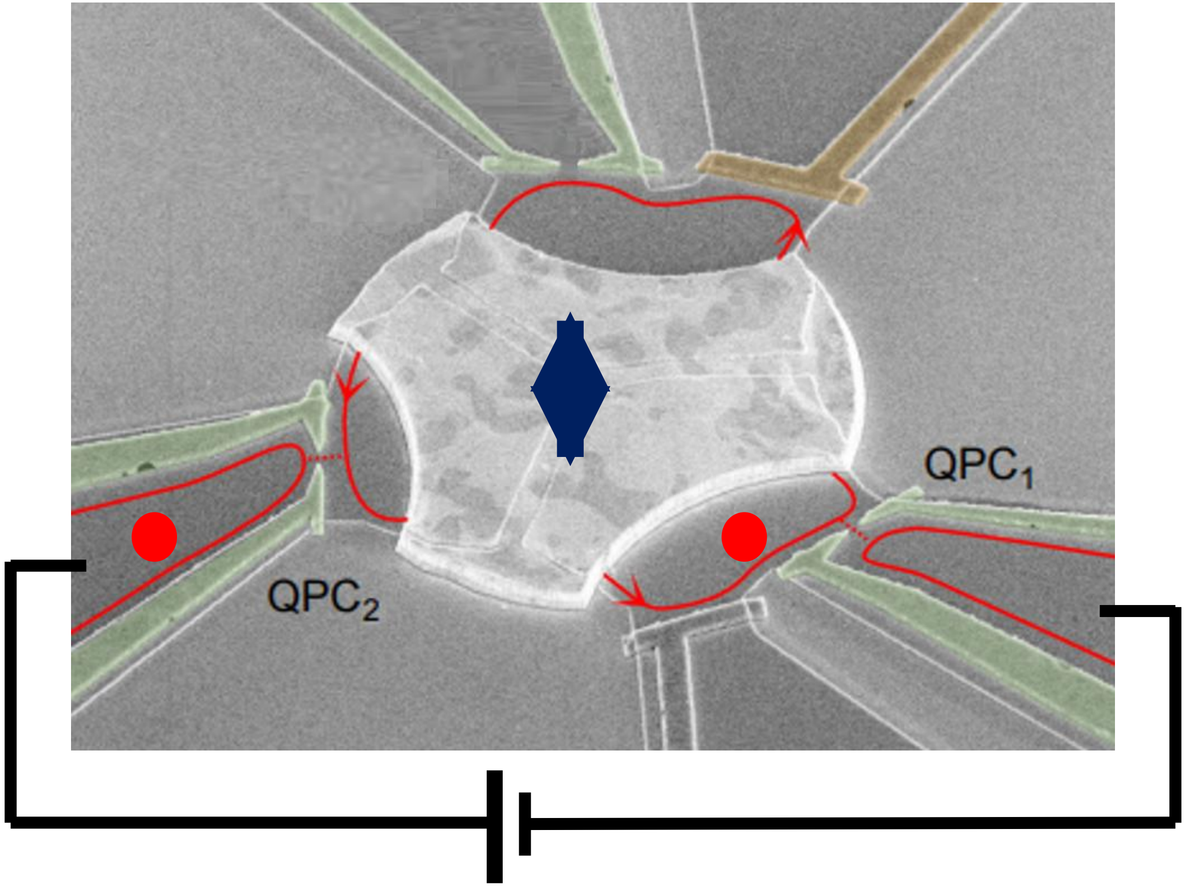


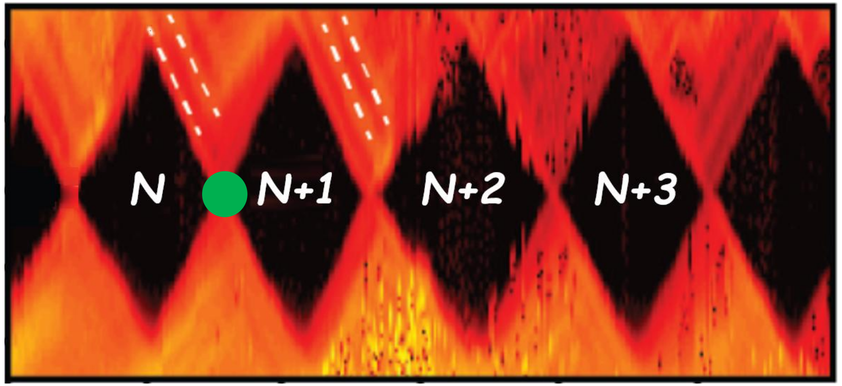
$$\left.\begin{array}{r} |N\rangle \equiv |\Downarrow\rangle \\ |N+1\rangle \equiv |\Uparrow\rangle \end{array}\right\}$$ QD charge qubit

Iftikhar *et al*, Nature 526, 233 (2015)

Iftikhar *et al*, Science, 360, 1315 (2018)

Large QDs: charge qubit





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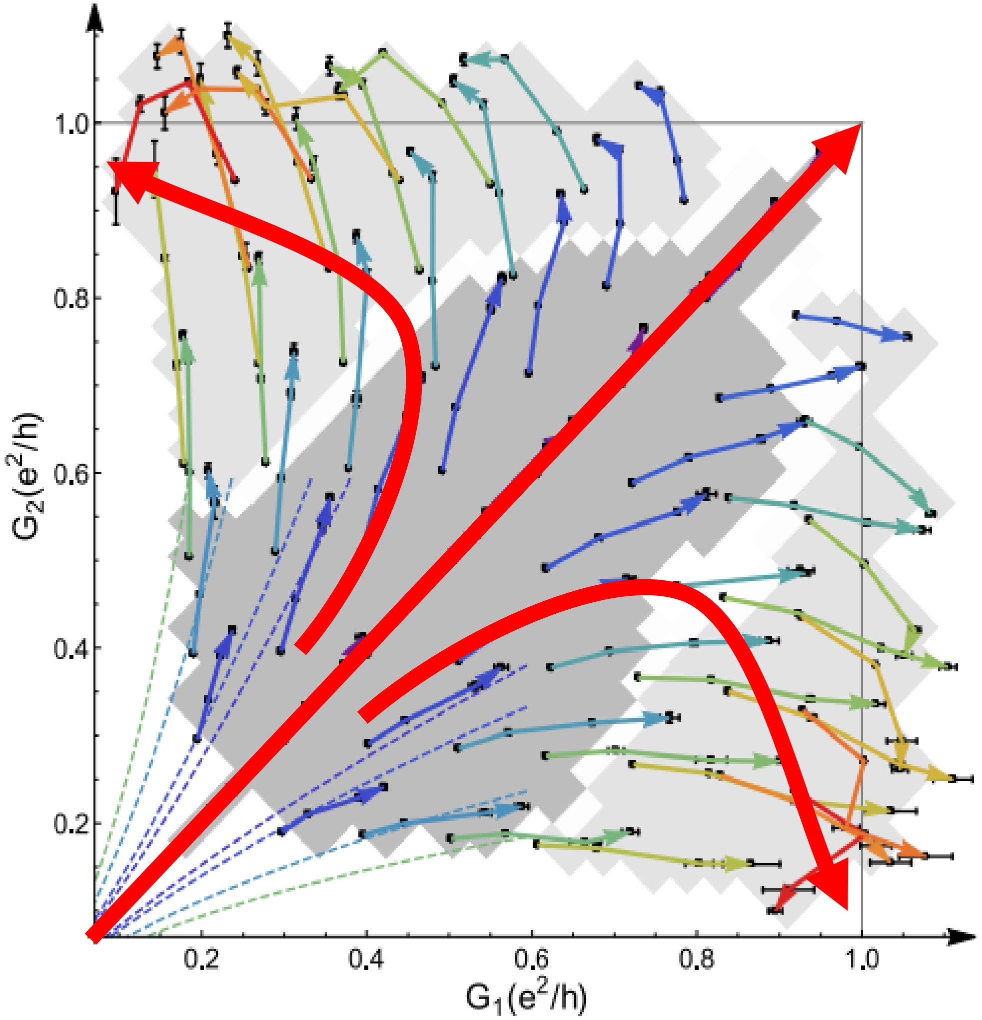
Boundary Quantum Criticality in QDs

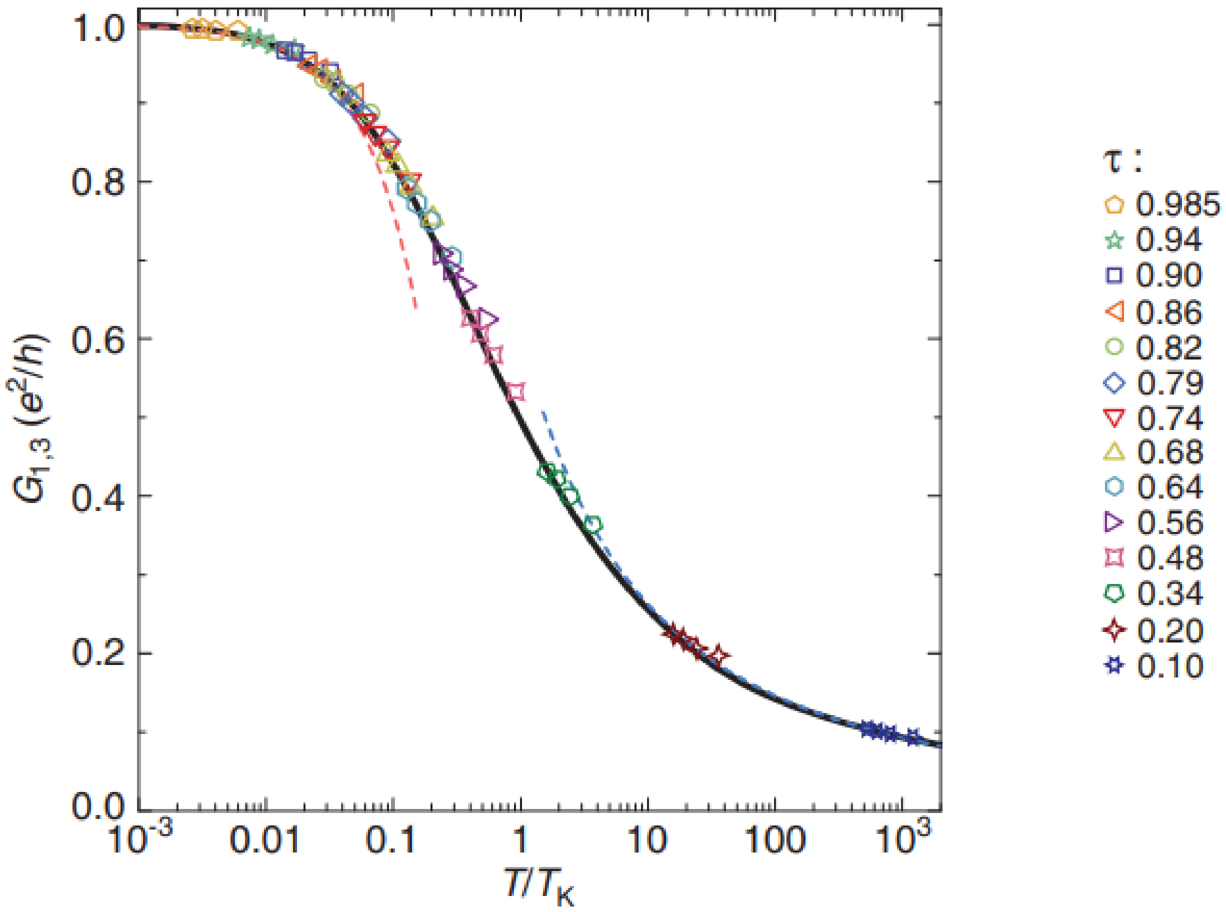
QD devices can realize nontrivial QPTs in a highly tunable setting



no complicated state preparation!

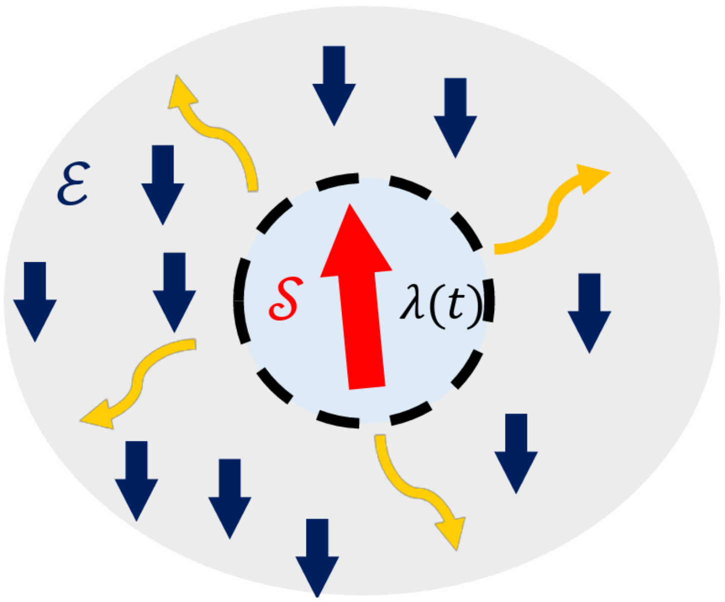
Iftikhar *et al*, Science, 360, 1315 (2018)

Electrical conductance: theory vs expt



Iftikhar *et al*, Science, 360, 1315 (2018)

Many-body system subject to driving



Open quantum system at equilibrium:

$$\hat{H}_0 = \hat{H}_S + \hat{H}_E + \hat{H}_{SE}$$

quantum dot

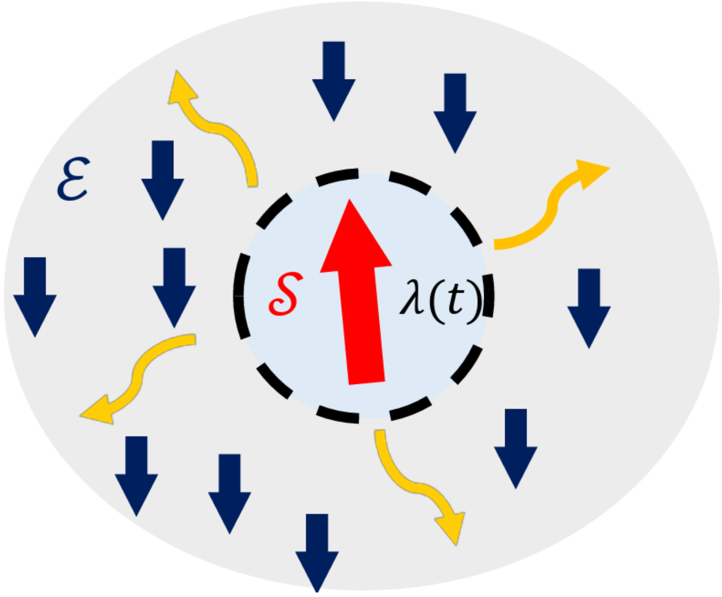
fermionic leads

dot-lead coupling

Finite-time driving:

$$\hat{H}_t = \hat{H}_0 + A\gamma(t)\,\hat{N}_S$$

Many-body system subject to driving



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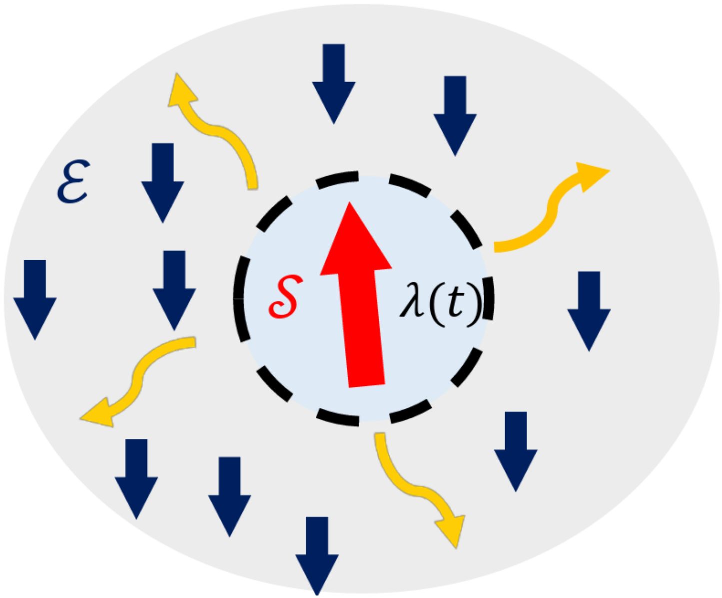
For QD devices: could be e.g. gate voltage (couples to QD charge) or magnetic field (couples to QD spin)

Many-body system subject to driving



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Example: linear ramp $\gamma(t) = t/\tau$

perturbation is applied for a finite duration τ through the ramp $\gamma(t)$ such that $\gamma(0) = 0$ and $\gamma(\tau) = 1$

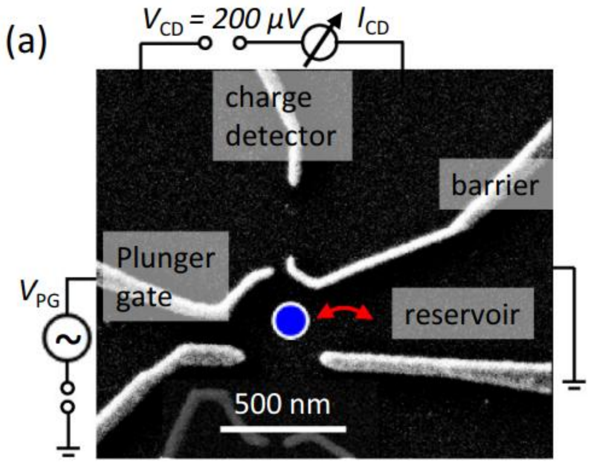
PHYSICAL REVIEW B **93**, 035425 (2016)

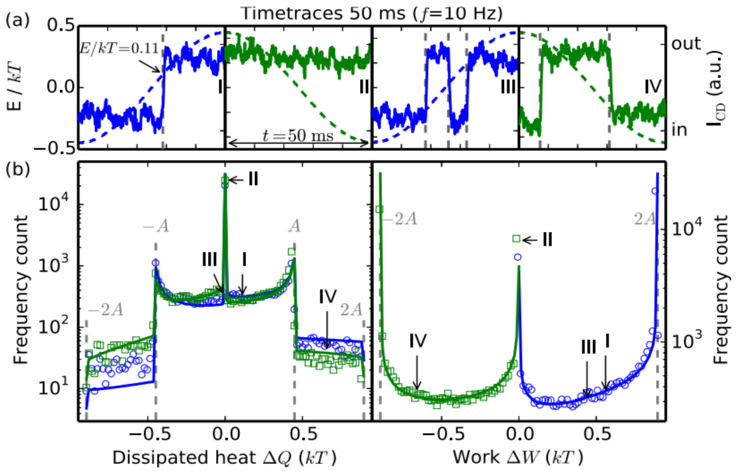
Equilibrium free energy measurement of a confined electron driven out of equilibrium

A. Hofmann,* V. F. Maisi, C. Rössler, J. Basset, T. Krähenmann, P. Märki, T. Ihn, K. Ensslin, C. Reichl, and W. Wegscheider
Solid State Physics Laboratory, ETH Zürich, 8093 Zürich, Switzerland

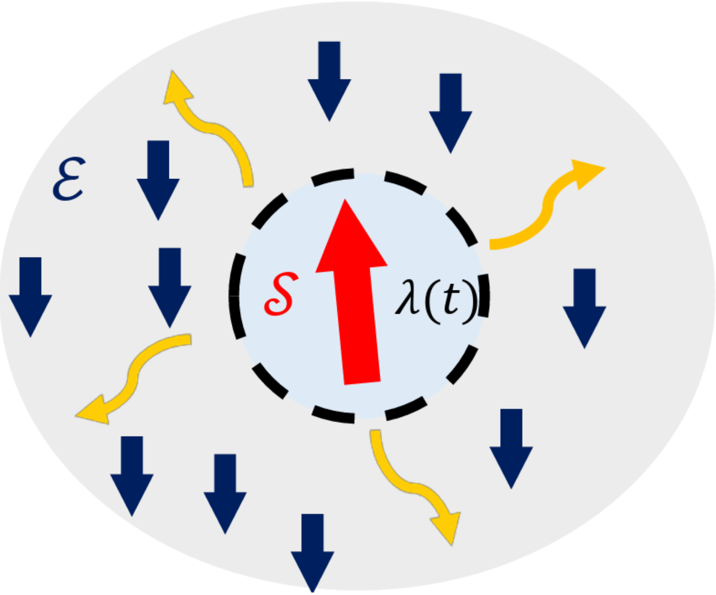
(Received 20 April 2015; revised manuscript received 2 November 2015; published 15 January 2016)

The Jarzynski equality relates nonequilibrium thermodynamics and equilibrium states. We realize a coupled quantum dot-electron reservoir system in which the time resolved observation of the tunneling dynamics is used to explicitly measure the exerted work and dissipated heat per single charge. We determine accurate values of the equilibrium free energy change over a large range of final state energies by driving the system far from equilibrium.





Quantum work distribution



Driven open quantum system

$$\hat{H}_0 = \hat{H}_S + \hat{H}_E + \hat{H}_{SE}$$

$$\hat{H}_t = \hat{H}_0 + A\gamma(t)\,\hat{N}_S$$

Two-point measurement (TPM) scheme:

$$P(W) = \sum_{m_\tau, n_0} \langle n_0|\rho_0|n_0\rangle \, p_{m_\tau|n_0} \, \delta(W - E_{m_\tau} + E_{n_0})$$

$$|\langle m_\tau|U_\tau|n_0\rangle|^2$$

Talkner, Lutz, Hanggi
PRE 75, 050102 (2007)

Linear Response Theory

PHYSICAL REVIEW LETTERS **133**, 070405 (2024)

Generalized Linear Response Theory for the Full Quantum Work Statistics

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[2] *Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, 14195 Berlin, Germany*
[3] *Department of Physics and Astronomy, The University of Manchester, Manchester M13 9PL, United Kingdom*

$$\chi_0(t) = i\theta(t)\mathrm{Tr}\{\hat{\rho}_0[\hat{N}_s(t), \hat{N}_s]\}$$

dynamical susceptibility

Ma, Sela, Mitchell
PRL 135, 130402 (2025)

$$\kappa_W^n = A^2 \int \frac{d\omega}{2\pi}\, \phi_n(\omega, T) R_\tau(\omega)\, \mathrm{Im}\chi_0(\omega)$$

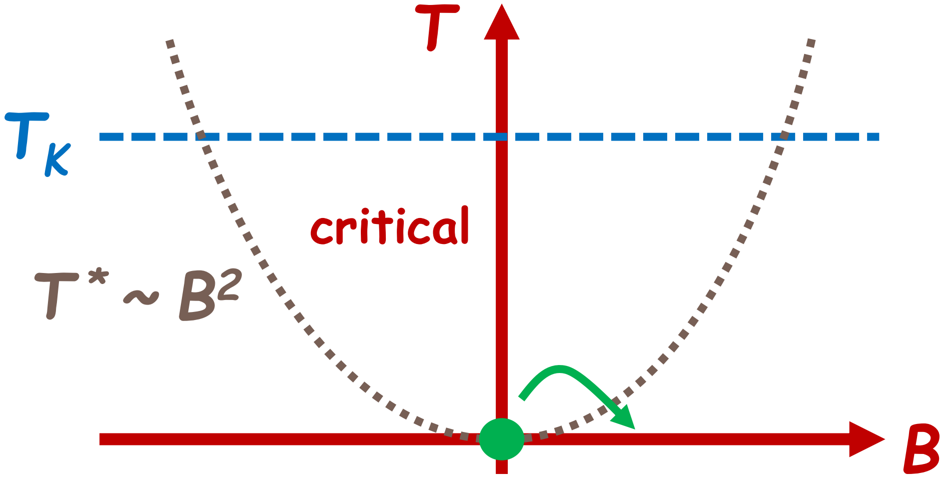
$$\phi_n(\omega, T) = \begin{cases} \omega^{n-2} & : n \text{ odd} \\ \omega^{n-2}\coth(\frac{\omega}{2T}) & : n \text{ even} \end{cases}$$

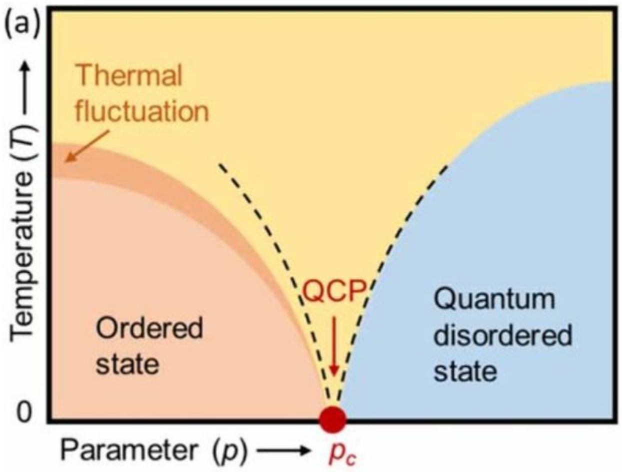
$$R_\tau(\omega) = \left|\int_0^\tau ds\, \dot{\gamma}(s) e^{-i\omega s}\right|^2$$

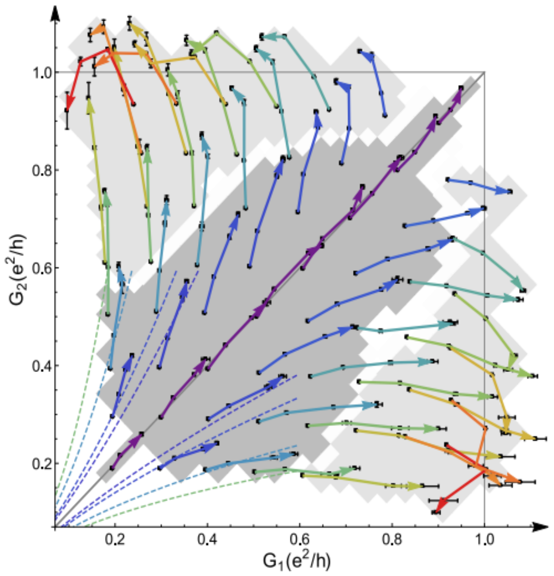
Perturbing a critical system

Prepare QD system at two-channel-Kondo quantum critical point

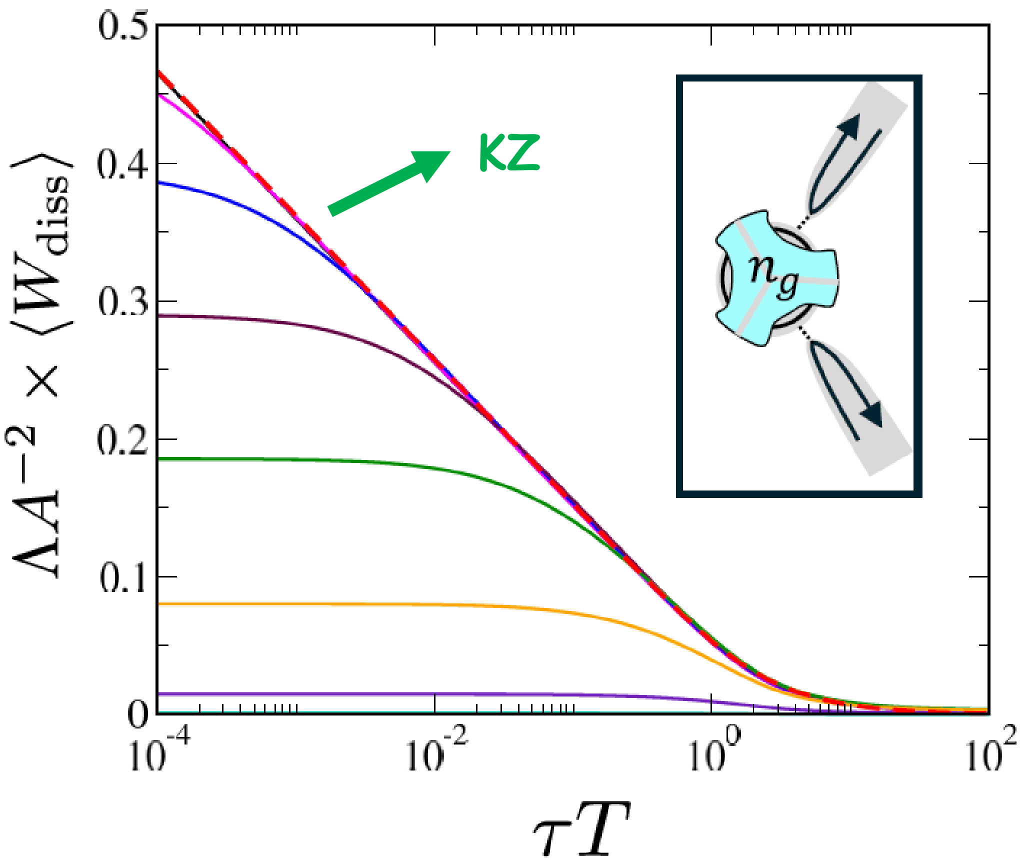
Apply a magnetic field B to the QD





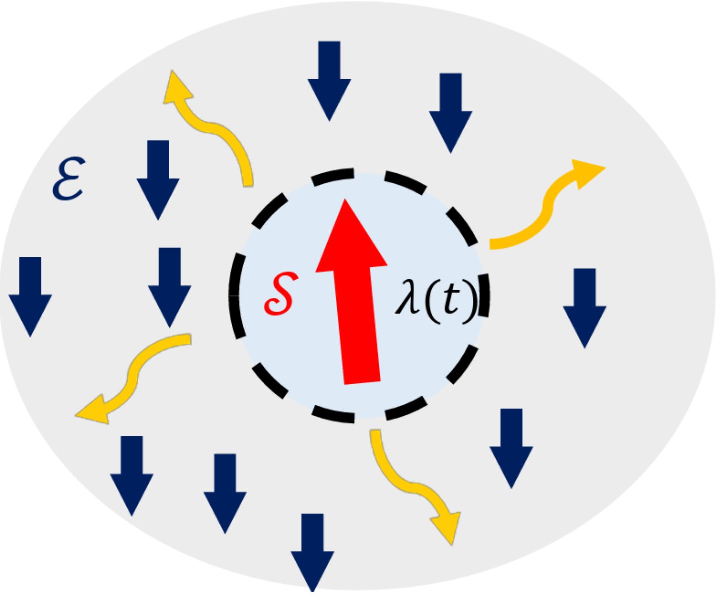


Dissipated Work in critical QDs



Ma, Sela, Mitchell PRL 135, 130402 (2025)

Work distribution function



Reconstruct full work distribution from cumulants in LR:

$$P(W) = P_0\delta(W) + \frac{A^2}{2\pi W^2}\left[1 + \coth\left(\frac{W}{2T}\right)\right] R_\tau(W)\, \mathrm{Im}\chi_0(W)$$

Universality near a QCP

relaxation function

$$\mathrm{Im}\chi_0(\omega) = \tfrac{1}{2}\omega T \int dt\, e^{i\omega t}\, \Psi_0(t)$$

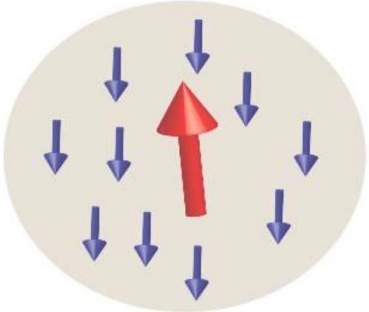
Scaling dimension of perturbation at QCP

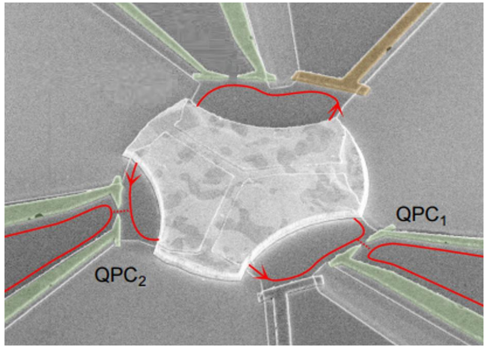
$$\Psi_0(t) = \beta \int_0^\beta ds\, \frac{1}{\Lambda^{2\Delta}} \left(\frac{\pi/\beta}{\sin \frac{\pi}{\beta}(s+it)} \right)^{2\Delta}$$

Determined by conformal invariance at QCP

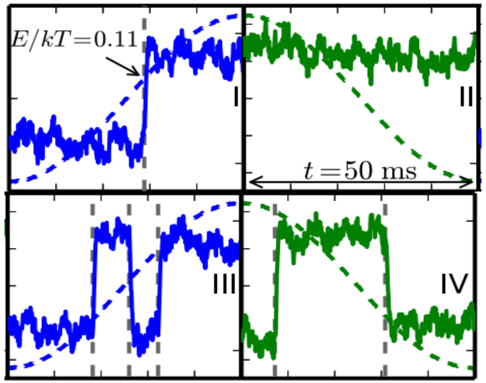
Conclusions

Quantum impurity models give a perspective on open quantum systems in strong coupling





Quantum nanoelectronic circuits are a versatile experimental platform for non-Markovian physics, including criticality



Dissipated work for driven systems can be computed exactly in the linear response limit