Quantum dots out of equilibrium
steady-state and quench dynamics

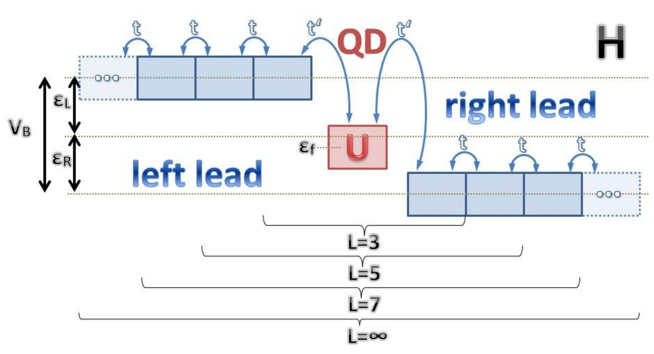
Graz University of Technology

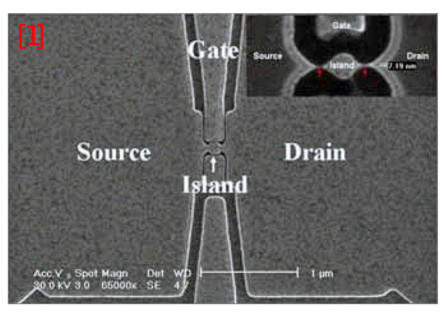
Martin Nuss, Martin Ganahl, Hans Gerd Evetz, Enrico Arrigoni, Wolfgang von der Linden
Institute of Theoretical and Computational Physics, Graz University of Technology, 8010 Graz, Austria
(martin.nuss@student.tugraz.at)

Model of a Quantum Dot

Quantum Dots

- **Out of equilibrium** situations: bias voltage, temperature gradients, ...
- ⇒ Nano- molecular electronics, quantum simulators, bio-physics
- **Charge** + **spin** fluctuations important
  ⇒ **many-body** effects (Kondo)





Single Impurity Anderson Model [2]

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_{\text{dot}} + \hat{\mathcal{H}}_{\text{lead}} + \hat{\mathcal{H}}_{\text{coup}}$$

$$\hat{\mathcal{H}}_{\text{dot}} = (-\frac{U}{2} + V_G) \sum_{\sigma} f_{\sigma}^{\dagger} f_{\sigma} + U \, \hat{n}_{\uparrow}^{f} \hat{n}_{\downarrow}^{f}$$

$$\hat{\mathcal{H}}_{\text{lead}} = \sum_{\alpha=\{L,R\}} \sum_{\sigma} \left(\epsilon^{\alpha} \sum_{i=0}^{\infty} c_{i\sigma}^{\alpha\dagger} c_{i\sigma}^{\alpha} - t \sum_{\langle i,j \rangle} c_{i\sigma}^{\alpha\dagger} c_{j\sigma}^{\alpha} \right)$$

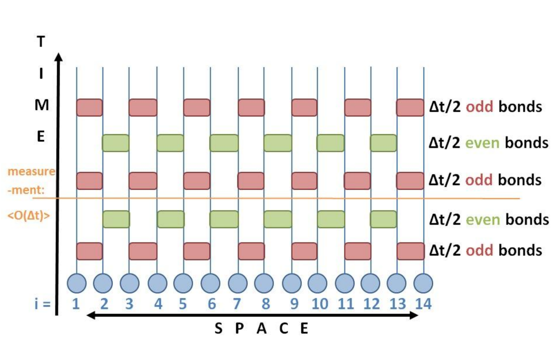
$$\hat{\mathcal{H}}_{\text{coup}} = -t' \sum_{\alpha=\{L,R\}} \sum_{\sigma} \left(c_{0\sigma}^{\alpha\dagger} f_{\sigma} + f_{\sigma}^{\dagger} c_{0\sigma}^{\alpha} \right)$$

- U ... dot on-site repulsion, t ... lead hopping integral
- $\epsilon^{L} = \mu^{L} = \frac{V_B}{2} = -\epsilon^{R} = -\mu^{R}$ ... V_B bias voltage
- V_G ... gate voltage, t' ... lead-dot coupling, $\Delta = \pi t'^2 \rho^{\alpha}(0)$

Real time evolution

Density Matrix Renormalization Group [3] + Time Evolving Block Decimation [4]

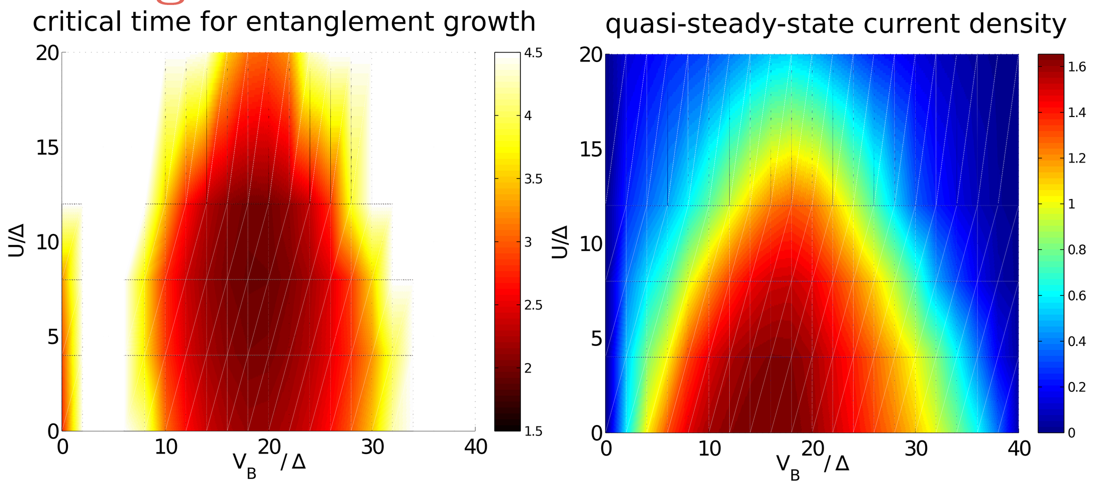
$$|\Psi\rangle = \sum_{\{s_1, s_2, \dots, s_L\}} c_{s_1, s_2, \dots, s_L} |s_1, s_2, \dots, s_L\rangle$$
$$= \sum_{\{s_1, \dots, s_L\}} \sum_{\{\alpha_1, \dots, \alpha_L\}} A_{\alpha_1}^{[1]s_1} A_{\alpha_1\alpha_2}^{[2]s_2} \dots A_{\alpha_{L-2}\alpha_{L-1}}^{[L-1]s_{L-1}} A_{\alpha_{L-1}}^{[L]s_L} |s_1, \dots, s_L\rangle$$



1. initial state DMRG($\hat{h}(\tau_0)$) ⇒ $|\Psi\rangle_0$
2. quench: $\hat{h} \to \hat{\mathcal{H}}$
3. time evolution
   TEBD($|\Psi\rangle(\tau)$) $= e^{-i\hbar\hat{\mathcal{H}}} |\Psi\rangle_0$

Entanglement ⇔ current

critical time for entanglement growth — quasi-steady-state current density



References

[1] C. S. Wu, Y. Makiuchi and C. Chen, InTech M. Wang (Ed.), 9789533070643 (1970).
[2] P. W. Anderson, Phys. Rev. **124**, 1 (1961).
[3] S. R. White Phys. Rev. B **48**, 14 (1993).
[4] G. Vidal Phys. Rev. Lett. **93**, 4 (2004).
[5] M. Potthoff, M. Aichhorn and C. Dahnken, Phys. Rev. Lett. **91**, 20 (2003).
[6] M. Balzer and M. Potthoff, Phys. Rev. B **83**, 19 (2011).
[7] M. Knap, W. von der Linden and E. Arrigoni, Phys. Rev. B **84**, 11 (2011).
[8] C. Gros and R. Valentí, Phys. Rev. B **48**, 1 (1993).
[9] A. C. Hewson, Cambridge University Press, 0521599474 (1997).
[10] M. Nuss, E. Arrigoni, M. Aichhorn and W.von der Linden, Phys. Rev. B **85**, 23 (2012).

3. Non-equilibrium Variational Cluster Approach (nVCA) [5–7]

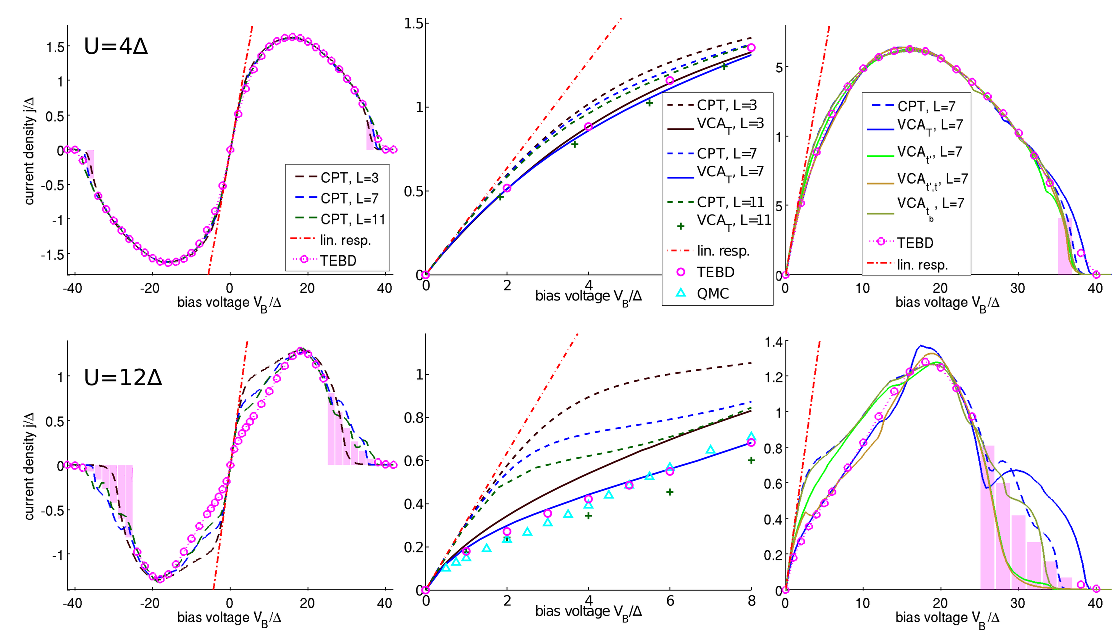
- Three **initially decoupled** systems (equilibrium): $\hat{h}$
  left lead - central region - right lead
  central region = **dot** + **parts of the leads**
- Full inifinite system $\hat{\mathcal{H}}$ (out of equilibrium):
  $$\hat{\mathcal{H}} = \hat{h} + \theta(\tau - \tau_0)\, \mathsf{T}\,.$$
- At some time τ_0 the **coupling** T **is switched on**.
- We are interested in the long-time, **steady-state** behavior
  ⇒time translation invariance: $\tau - \tau' \to \omega$
- **Keldysh** Green's function - formalism:
  $$\widetilde{\mathsf{G}}(\omega) = \begin{pmatrix} \mathsf{G}^{\mathsf{R}}(\omega) & \mathsf{G}^{\mathsf{K}}(\omega, \mu) \\ 0 & \mathsf{G}^{\mathsf{A}}(\omega) \end{pmatrix}$$
- $\mathsf{g}^{\mathsf{R/A}}$ of $\hat{h}$ by
  - **analytical form** for non-interacting **leads**
  - **exact diagonalization** (Band-Lanczos) for **central**, interacting region
- $\mathsf{g}^{\mathsf{K}}(\omega, \mu)$ of $\hat{h}$ (equilibrium) by
  $$\mathsf{g}^{\mathsf{K}}(\omega, \mu) = \left(\mathsf{g}^{\mathsf{R}}(\omega) - \mathsf{g}^{\mathsf{A}}(\omega)\right)\,(1 - 2p_{\text{FD}}(\omega, \mu, \beta))$$
  - $p_{\text{FD}}(\omega, \mu, \beta)$ ... Fermi-Dirac distribution
- Steady-state $\widetilde{\mathsf{G}}(\omega)$ of $\hat{\mathcal{H}}$ via Cluster Perturbation Theory (**CPT**) [8]
  $$\widetilde{\mathsf{G}}^{-1} = \widetilde{\mathsf{g}}^{-1} - \widetilde{\mathsf{T}}$$
- First order strong coupling perturbation theory in T
  - approximation: **self-energy** $\Sigma_{\hat{\mathcal{H}}} \stackrel{!}{=} \Sigma_{\hat{h}}$
- **exact limits**: $L \to \infty$, $U \to 0$, $\frac{U}{t} \to \infty$
- Improve starting point of calculation by **variational feedback** [7] of steady-state target onto initial state
  - add **single-particle fields** $\hat{\Delta}(\mathsf{x})$ before τ_0:
    $\hat{h} \mapsto \hat{h} + \sum_i \mathsf{x}_i \hat{\Delta}_i$
  - subtract them again after coupling: $\mathsf{T} \mapsto \mathsf{T} - \sum_i \mathsf{x}_i \Delta_i$
  - ⇒ flexible $\Sigma(\mathsf{x})$
  - variational principle: $\langle \hat{\Delta}_i \rangle_{\text{initial-state}} \stackrel{!}{=} \langle \hat{\Delta}_i \rangle_{\text{steady-state}}$
- Steady-state **current-density**:
  $$j_{ij} = \frac{t_{ij}}{2} \sum_{\sigma} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \Re\mathrm{e}\left(\mathsf{G}_{ij}^{\mathsf{K}}(w) - \mathsf{G}_{ji}^{\mathsf{K}}(w)\right)$$
- Non-equilibrium local **density of states** (nLDOS):
  $$\rho_f(\omega) = -\frac{1}{\pi} \sum_{\sigma} \Im\mathrm{m}\left(\mathsf{G}_{ff}^{\mathsf{R}}(w)\right)$$

Conclusions

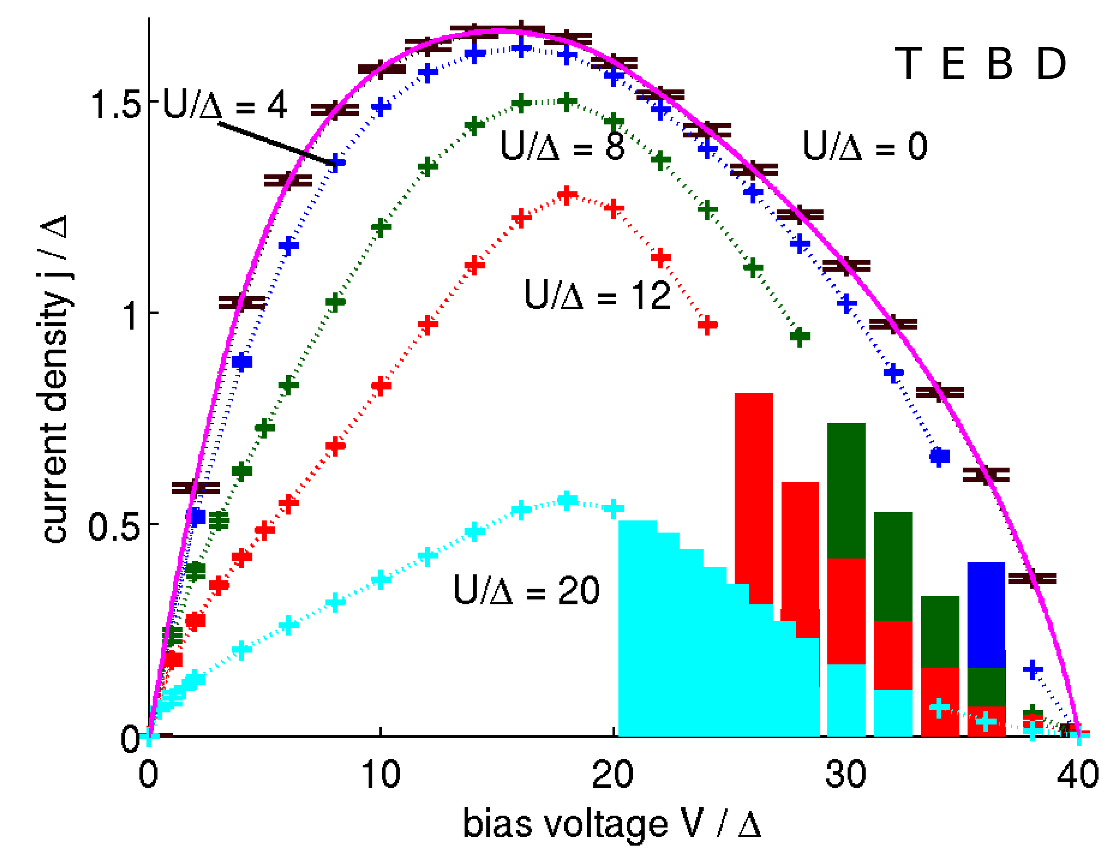
- Quantum dot **steady-state: nVCA**
  - **very good current density** up to intermediate U
  - **agrees with TEBD benchmark** (≤ interm. V_B)
  - **linear splitting of Kondo resonance** in nLDOS
  - **Kondo regime + Coulomb blockade**
  - nVCA ≫ nCPT ⇒ **variational feedback crucial**
- Quantum dot **quench** dynamics: **TEBD**
  - **quasi-steady-state plateau** (like TD limit)
  - **current density** correlates with **entanglement**
  - **different quenches ⇒ same steady-state** but different **quality** of the plateaus
  - **charge and spin** dynamics seperate

Results

Current-voltage characteristics

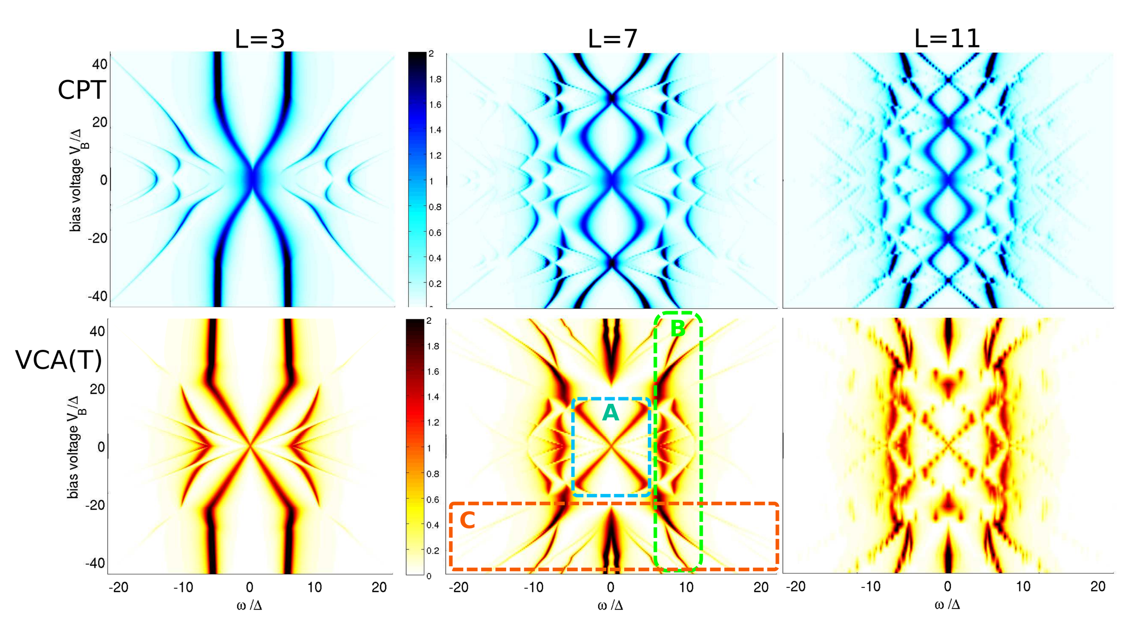


- nVCA ≫ nCPT, linear response, lead-band effects



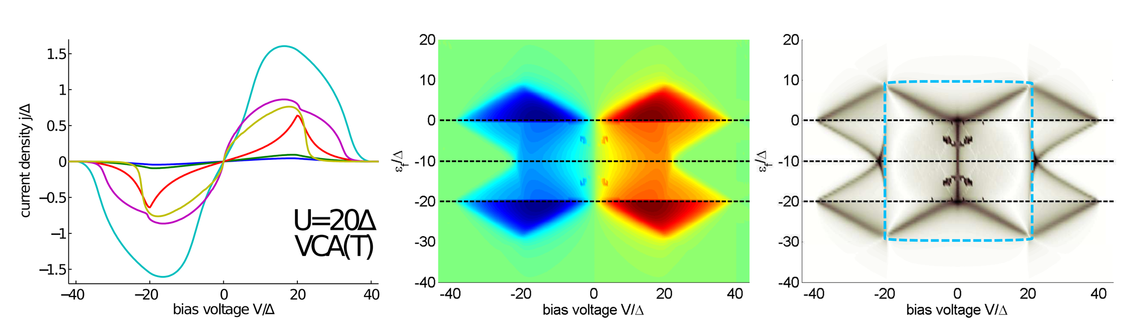
- TEBD quasi-exact, some bias regions upper bounds

Non-equilibrium local density of states



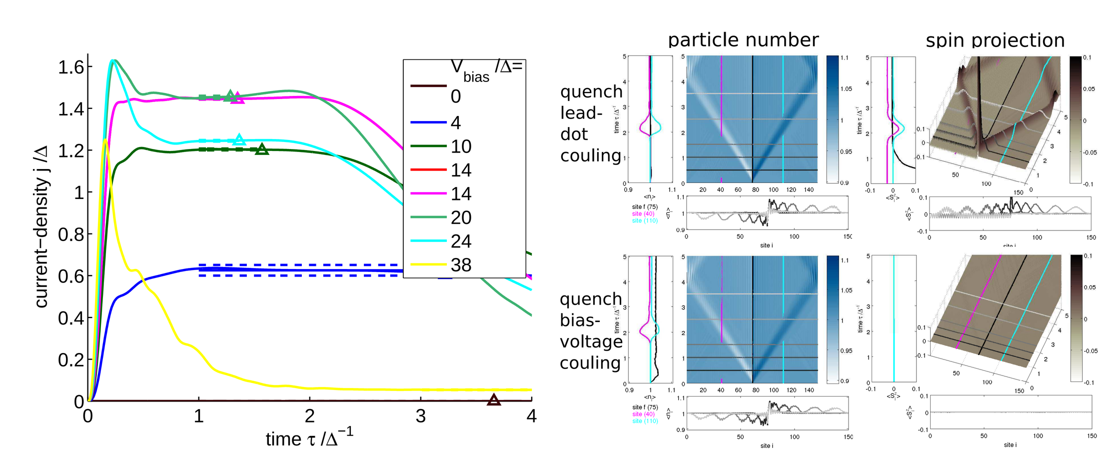
- linear splitting of Kondo resonance
- merging with Hubbard bands

Effects of a gate voltage: stability diagram



- Kondo effect [9, 10]
- Coulomb blockade

Time evolution of current, charge, spin



- TEBD reaches quasi-steady-state plateau
- particle and spin dynamics seperate

MN acknowledges support of the Austrian Science Fund (FWF) P24081 and SFB ViCoM projects F04103 and F04104. Parts of the caluclations were done on the vienna scientific cluster.