Nonequilibrium Kondo effect in a magnetic field: Auxiliary master equation approach

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Kondo effect

Figure: Quantum dot: (a,b) Schematic view, (c) SEM image.[1,2]

- Resonant spin-flip scattering at $\omega \approx \mu$
- Kondo resonance in spectral function $A(\omega)$ with width $\approx 2T_K$
- Kondo scale T_K exponentially small
- All energy scales $T, \phi, B, \ldots \ll T_K$

➡ Hard to adress numerically!

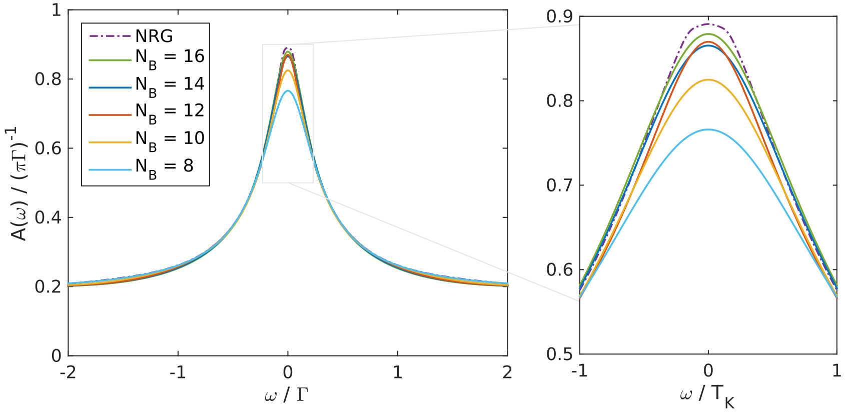

Figure: Comparison to NRG.[3]

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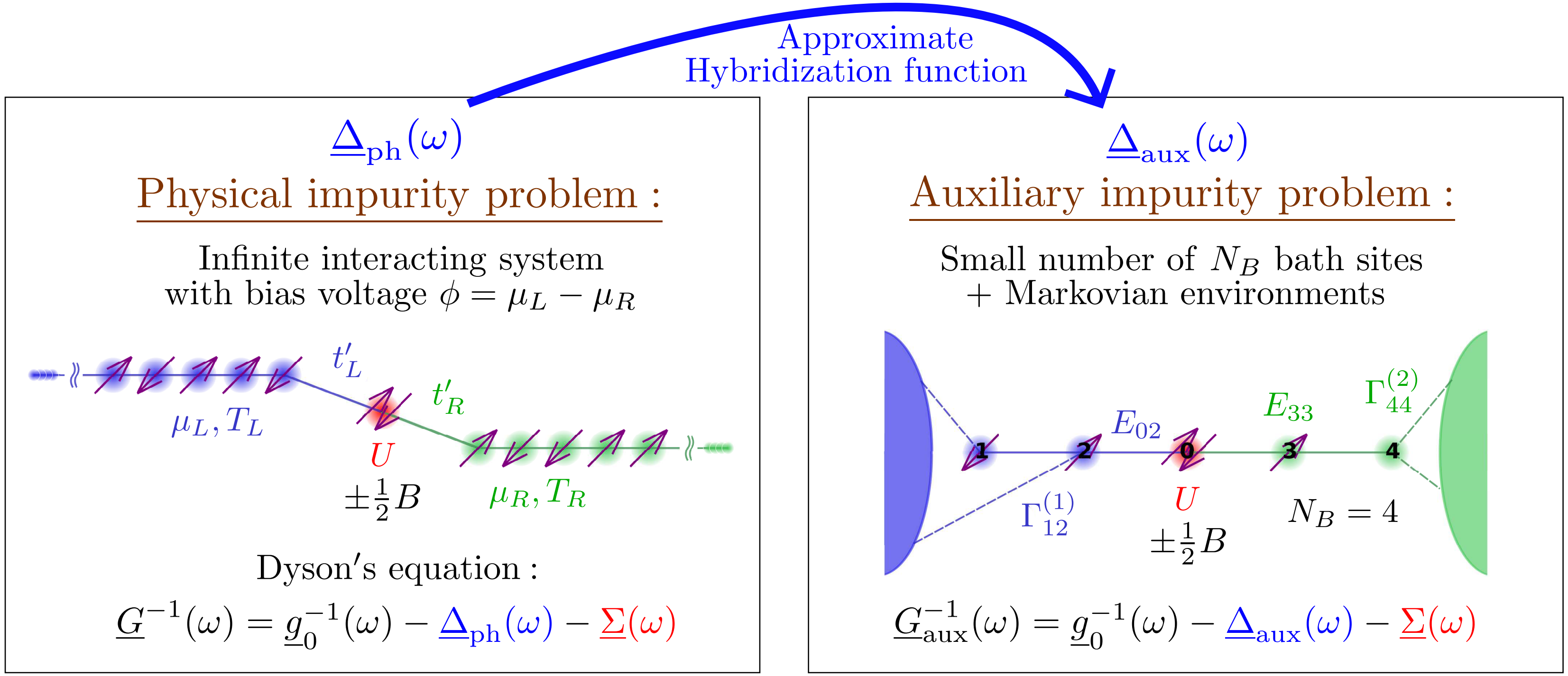
[1] D. Goldhaber-Gordon *et al.*, Nature 391, 156 (1998)

[2] S. De Franceschi *et al.*, in Handbook of Nanophysics (CRC, 2010), pp.646-664

[3] A. Dorda *et al.*, PRB 92, 125145 (2015)

Method: Auxiliary master equation approach [1]



Approximate Hybridization function

$\underline{\Delta}_{\mathrm{ph}}(\omega)$

Physical impurity problem :

Infinite interacting system with bias voltage $\phi = \mu_L - \mu_R$

Dyson's equation :

$$\underline{G}^{-1}(\omega) = \underline{g}_0^{-1}(\omega) - \underline{\Delta}_{\mathrm{ph}}(\omega) - \underline{\Sigma}(\omega)$$

$\underline{\Delta}_{\mathrm{aux}}(\omega)$

Auxiliary impurity problem :

Small number of N_B bath sites + Markovian environments

$$\underline{G}_{\mathrm{aux}}^{-1}(\omega) = \underline{g}_0^{-1}(\omega) - \underline{\Delta}_{\mathrm{aux}}(\omega) - \underline{\Sigma}(\omega)$$

- Dynamics governed by the Lindblad equation:

$$\frac{d\rho}{dt} = \mathcal{L}\rho = (\mathcal{L}_H + \mathcal{L}_D)\,\rho$$

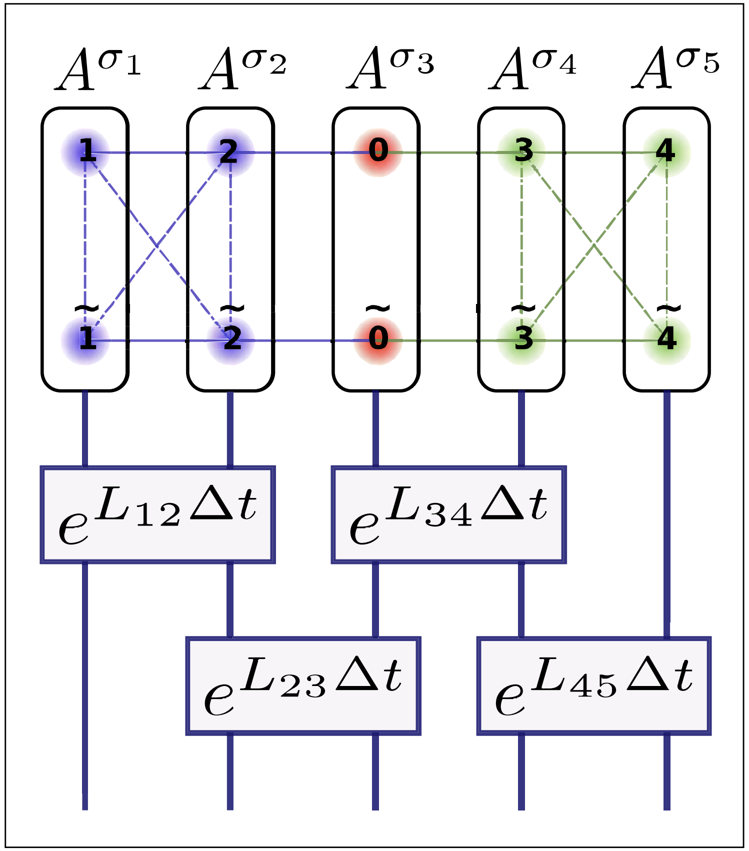
$$\mathcal{L}_H\rho = -i[H_{aux}, \rho]\,, \qquad H_{aux} = \sum_{n,m,\sigma} E_{nm} c^\dagger_{n\sigma} c_{m\sigma} + U n_{0\uparrow} n_{0\downarrow} - B S_{0z}$$

$$\mathcal{L}_D\rho = \sum_{n,m,\sigma} \left[\Gamma^{(1)}_{nm} \left(c_{n\sigma}\rho c^\dagger_{m\sigma} - \tfrac{1}{2}\{c^\dagger_{m\sigma}c_{n\sigma}, \rho\} \right) + \Gamma^{(2)}_{nm} \left(c^\dagger_{n\sigma}\rho c_{m\sigma} - \tfrac{1}{2}\{c_{m\sigma}c^\dagger_{n\sigma}, \rho\} \right) \right]$$

- Contains fit parameters for the mapping
- Exponentially exact for $N_B \to \infty$

Solution: Time evolving block decimation [2]

- Super-fermion representation [3]
  $\hat{\rho} \rightarrow |\rho\rangle$ in a larger state space
- State vector as MPS [4,5]
  $$|\rho\rangle = \sum_{\{\sigma_i\}} c_{\{\sigma_i\}} |\{\sigma_i\}\rangle = \sum_{\{\sigma_i\}} \boldsymbol{A}^{\sigma_1}\boldsymbol{A}^{\sigma_2}\boldsymbol{A}^{\sigma_3}\boldsymbol{A}^{\sigma_4}\boldsymbol{A}^{\sigma_5} |\{\sigma_i\}\rangle$$
- Time evolution $\quad |\rho(t)\rangle = e^{Lt}|\rho(0)\rangle$
  Steady state $\quad L|\rho_\infty\rangle = 0$
- Trotter decomposition
  $$e^{L\Delta t} = e^{L_e \Delta t} e^{L_o \Delta t} + \mathcal{O}(\Delta t^2)$$
- Steady state, Green's functions, ...



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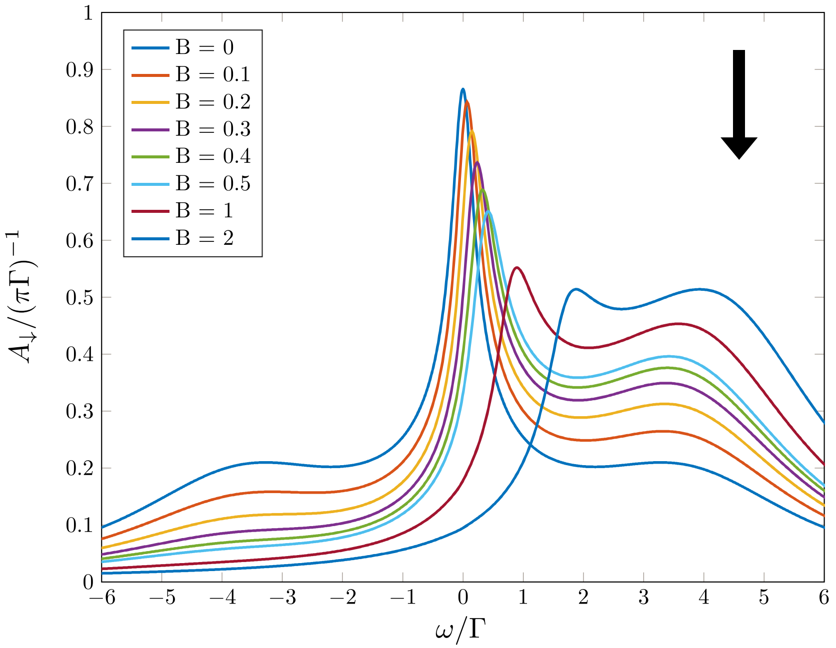
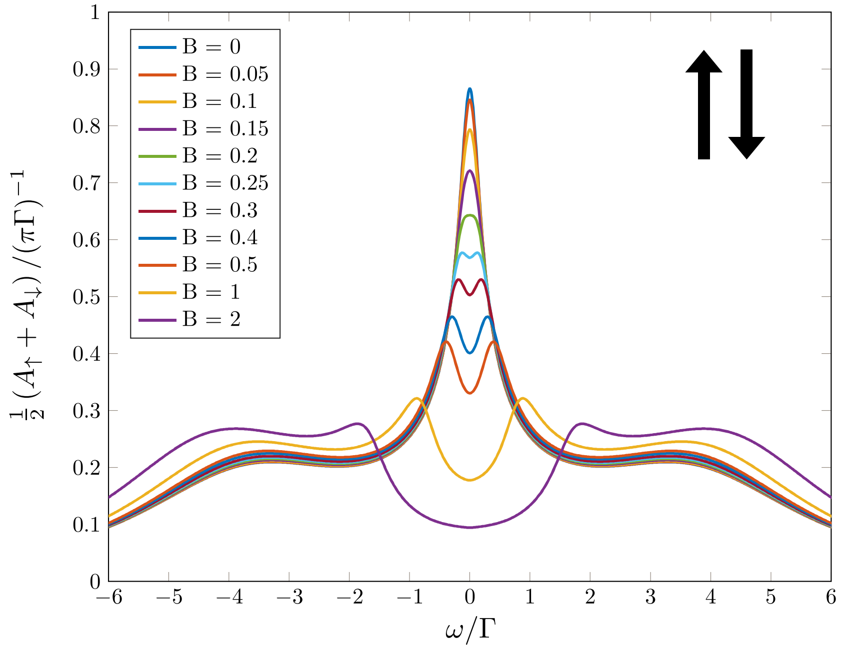
[1] A. Dorda *et al.*, PRB 89, 165105 (2014)
[2] G. Vidal, PRL 93, 040502 (2004)
[3] A. Dzhioev *et al.*, J. Chem. Phys. 134, 044121 (2011)
[4] U. Schollwöck, Annals of Physics 326, 96 (2011)
[5] A. Dorda *et al.*, PRB 92, 125145 (2015)

Spectral function

Equilibrium, $\phi = 0$



$U = 6\Gamma,\ T = 0.05\Gamma,\ T_K \approx 0.2\Gamma$

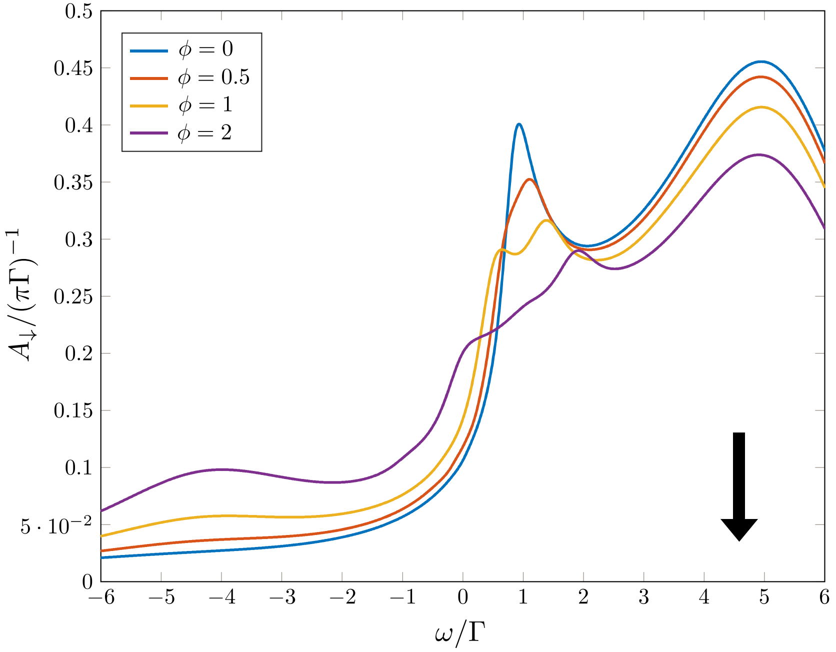


Effect of a magnetic field:

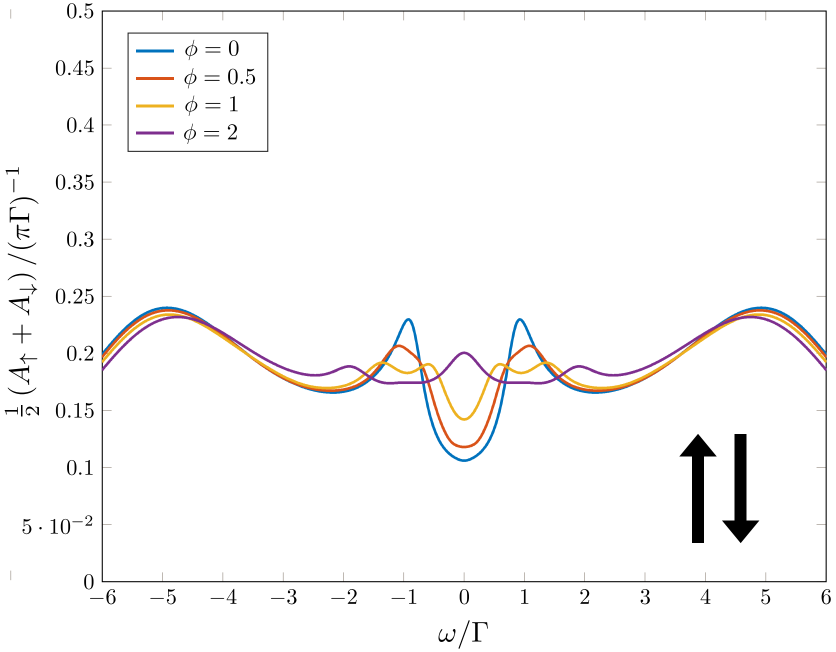
- Different spectral functions $A_\uparrow(\omega) = A_\downarrow(-\omega)$
- Suppression, broadening and shift/splitting of the Kondo resonance
- Splitting at $B \gtrsim T_K$ between B and $2B$

Spectral function

Nonequilibrium, $\phi > 0$



$U = 8\Gamma, \; T = 0.05\Gamma, \; T_K \approx 0.1\Gamma, \; B = \Gamma$

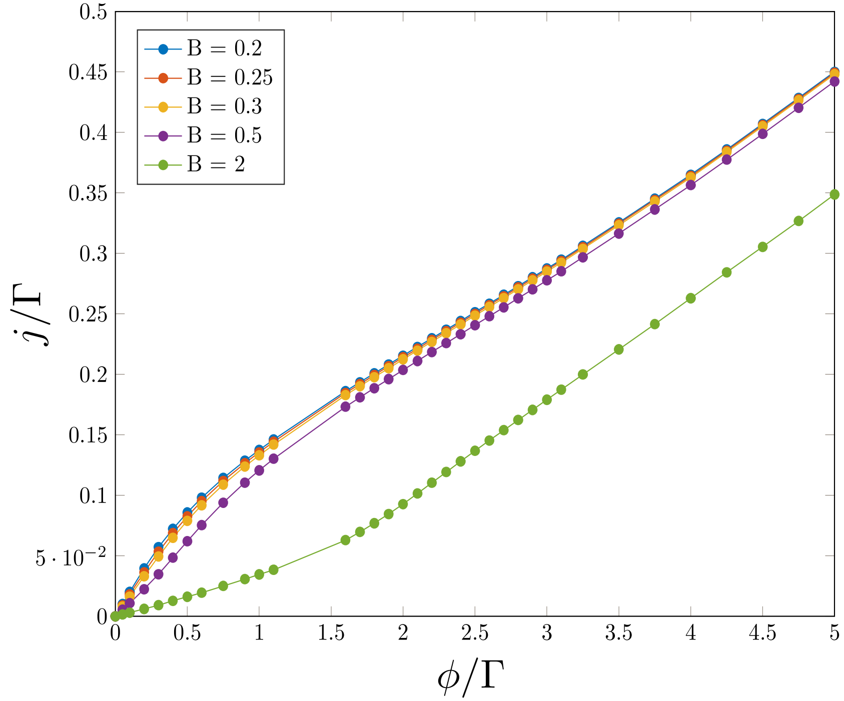


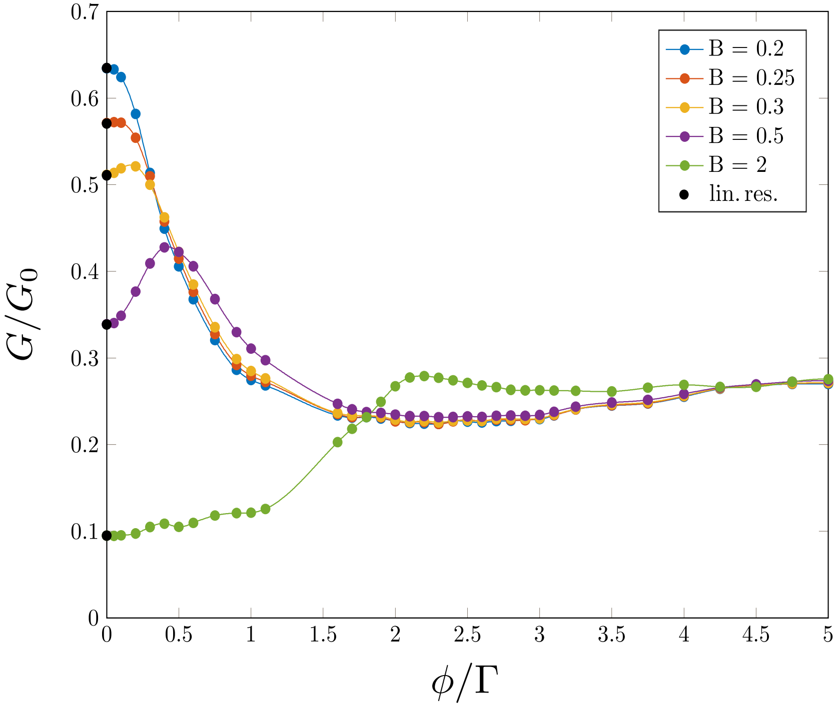
Effect of a bias voltage:

- Suppression, broadening and splitting of the Kondo resonance
- Symmetric for $B = 0$, asymmetric for finite B
- 4-peak structure in total spectrum for certain parameters

Current & differential conductance

$U = 6\Gamma,\ T = 0.05\Gamma,\ T_K \approx 0.2\Gamma$

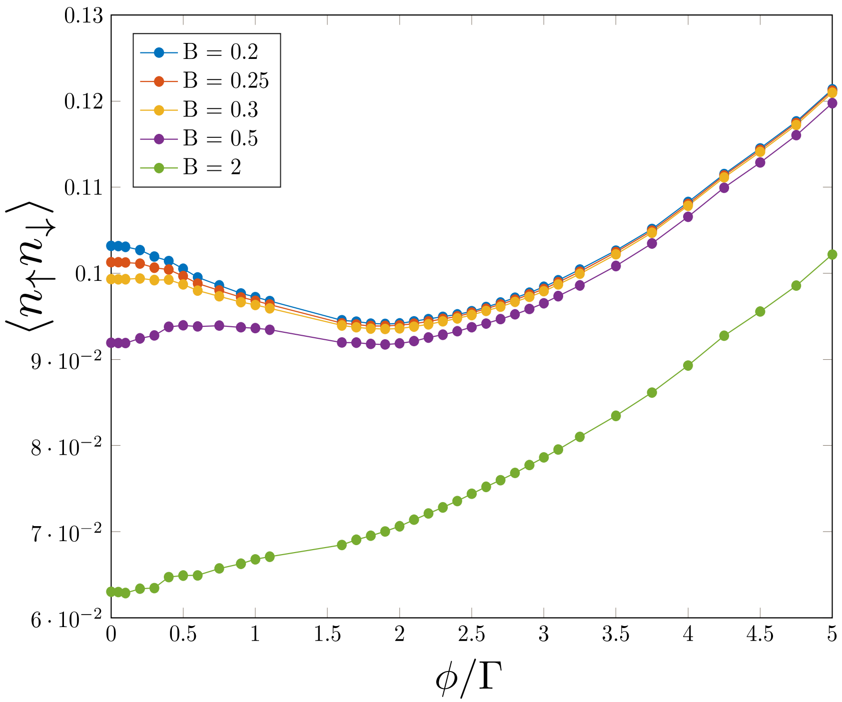


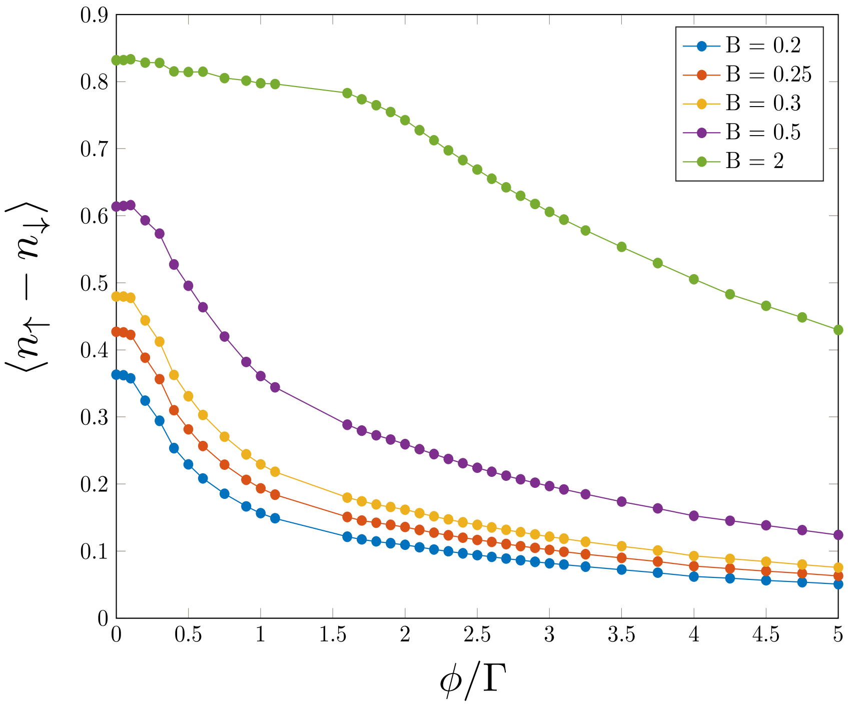


- Delayed Kondo shift in the differential conductance
- Similar linear current-voltage characteristics at large bias

Double occupancy, magnetization

$U = 6\Gamma,\ T = 0.05\Gamma,\ T_K \approx 0.2\Gamma$





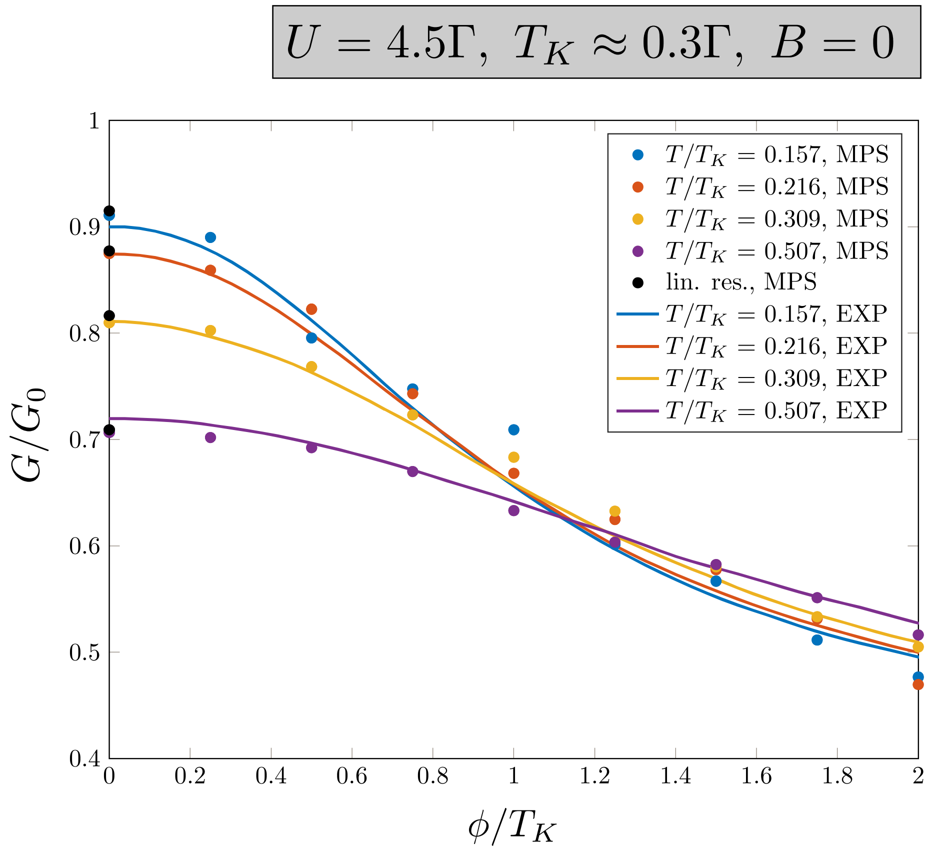
Double occupancy:

- Delayed Kondo shift, similar to the differential conductance
- Minimum for small B, increase by enlarged transport window

Magnetization:

- Plateau until $\phi \lesssim B$ for large B, decrease

Comparison to recent experiments



$U = 4.5\Gamma,\ T_K \approx 0.3\Gamma,\ B = 0$

- Quantum dot realized in an InAs nanowire [1,2]
- Nice agreement to the experiment also outside the Kondo regime

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[1] A.V. Kretinin *et al.*, PRB 84, 245316 (2011)

[2] A.V. Kretinin *et al.*, PRB 85, 201301 (2012)

Thanks for your attention!

Other works on the Kondo effect in a magnetic field:

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[1] J. E. Moore *et al.*, PRL 85, 1722 (2000)
[2] T. A. Costi, PRL 85, 1504 (2000)
[3] F. B. Anders, PRL 101, 066804 (2008)
[4] A. Dirks *et al.*, EPL 102, 37011 (2013)
[5] A. Rosch *et al.*, PRL 90, 076804 (2003)
[6] M. Fritsch *et al.*, PRB 81, 035113 (2010)
[7] S. Smirnov *et al.*, New Journal of Physics 15, 073047 (2013)
[8] I. J. Hamad *et al.*, PRB 92, 195113 (2015)