Numerical renormalization group part 5

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When things go wrong

- Code doesn't start at all. Library problems? Wrong CPU optimization?
- No Mathematica licence available (in network licence environments).
- Typos in input file. Case is important. Spaces are important.
- Errors in model definition file (code is not valid Mathematica language code).
- Convergence? Increase truncation cutoffs, if memory/time allows.
- Suitable Λ? Too small, too large?
- Wrong `symtype`
- Truncation within clusters (`safeguard`)
- Floating-point errors (`fixeps`)
- Inappropriate `Tmin` (should be some orders of magnitude smaller than the lowest energy scale in the problem)

...CONTINUED

- Model parameters must be in [extra] block, NRG parameters in [param] block
- Model definition is not what you think it is.
- Path problems (files are not where you think they are)
- Operators used in `specd` missing in `ops`
- Inappropriate broadening parameter (N_z vs α)
- Confusion between `T` (physical parameter) and `Tmin` (chain length)
- Too slow? Are parameters sensible? Use parallelization.
- Running out of disk space during calculation? Set `workdir`.

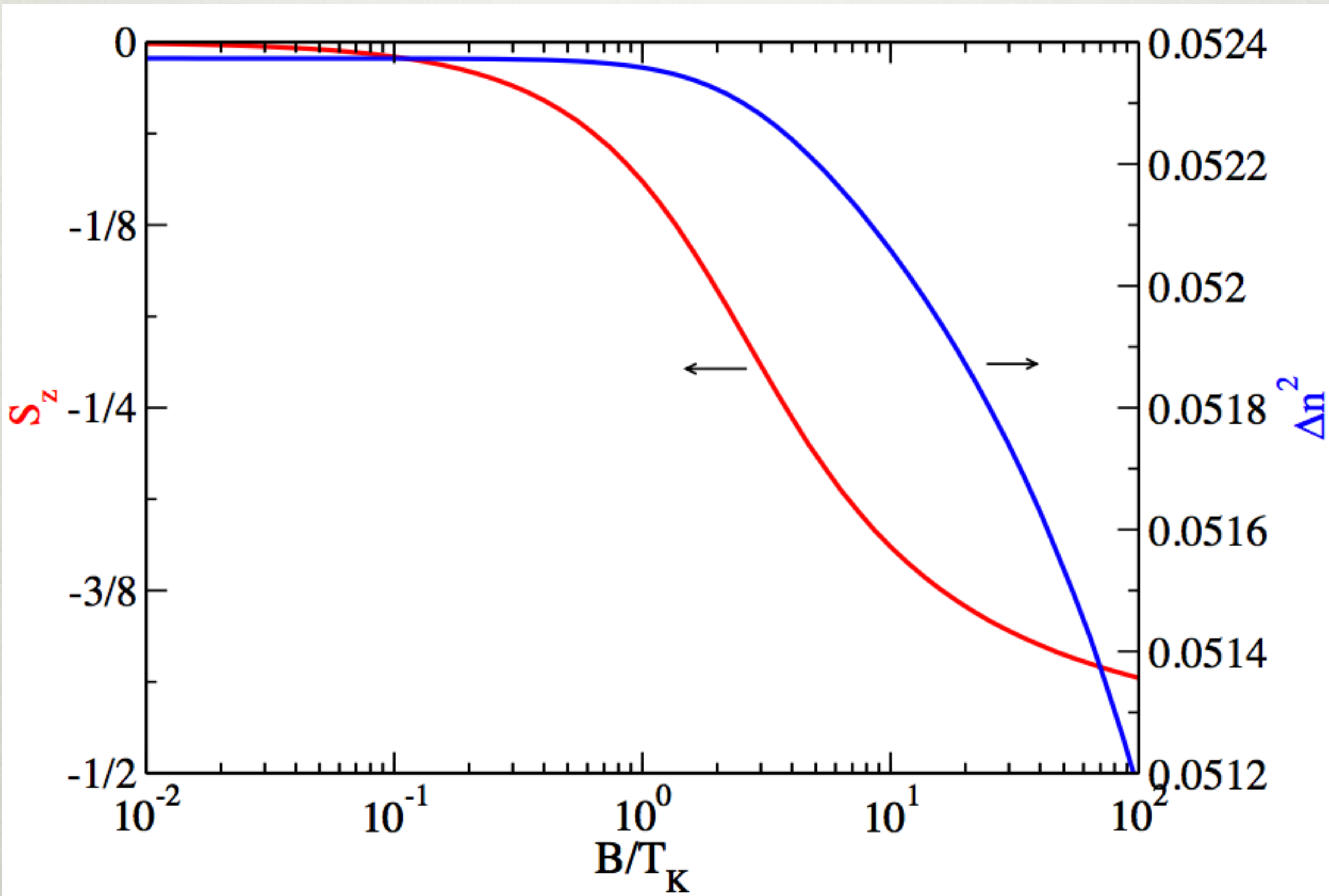
Troubleshooting

- Run code manually, without scripts. Call `nrginit` and `nrgrun` separately.
- Inspect log files (`mmalog`, `log`).
- Increase the verbosity of output (`log=` setting, see `param.cc` for documentation).
- Do results make physical sense?
- Check the details (sum rules, compare with different methods, etc.)
- If the results are "interesting", check twice! Then check again!

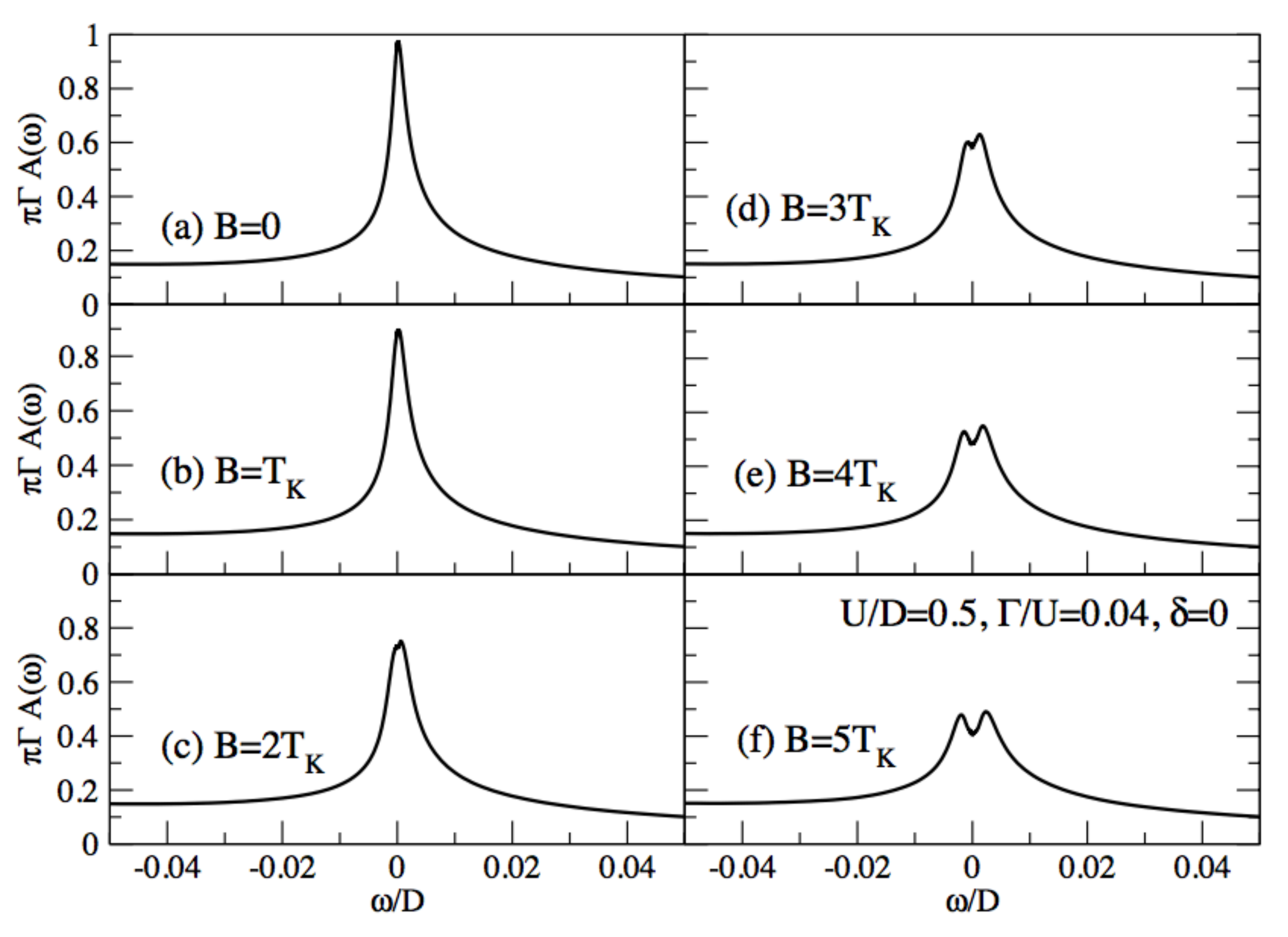
Good to know

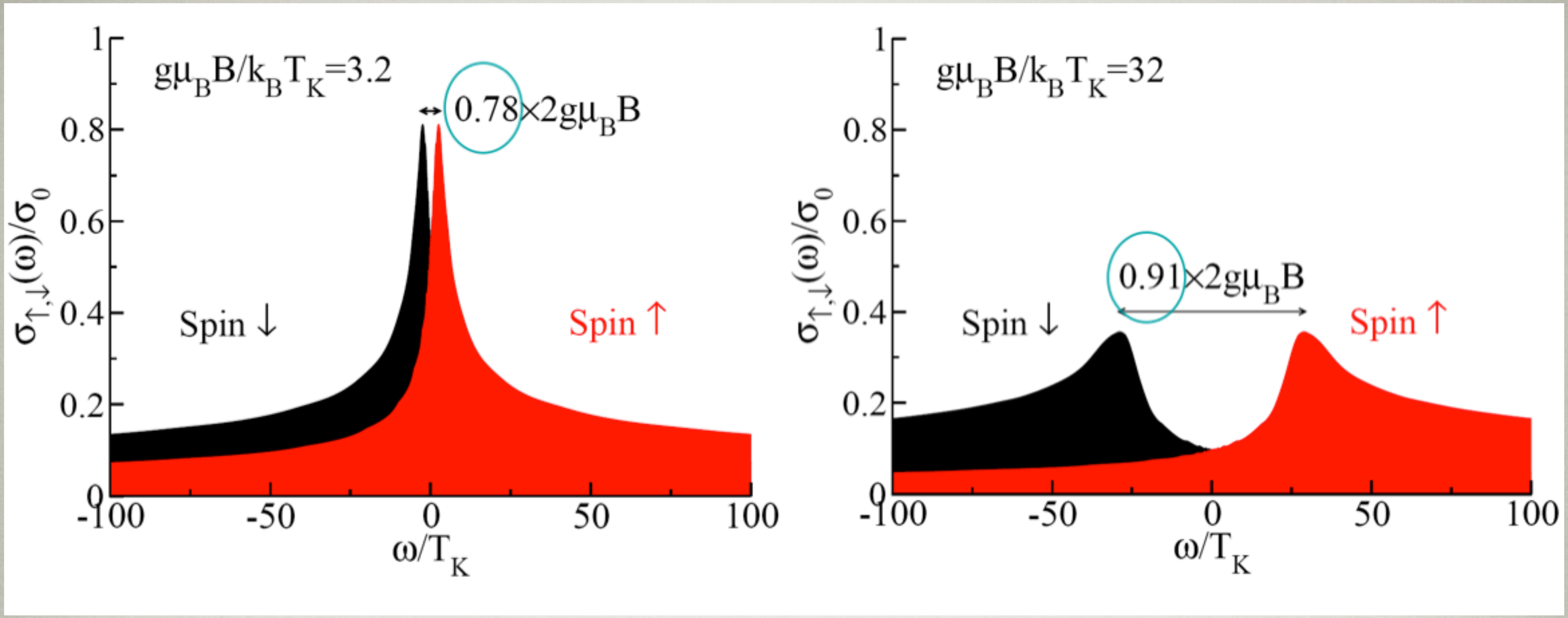
- Interleaved iteration (`substeps=true`)
- Different unit? Use `bandrescale`
-

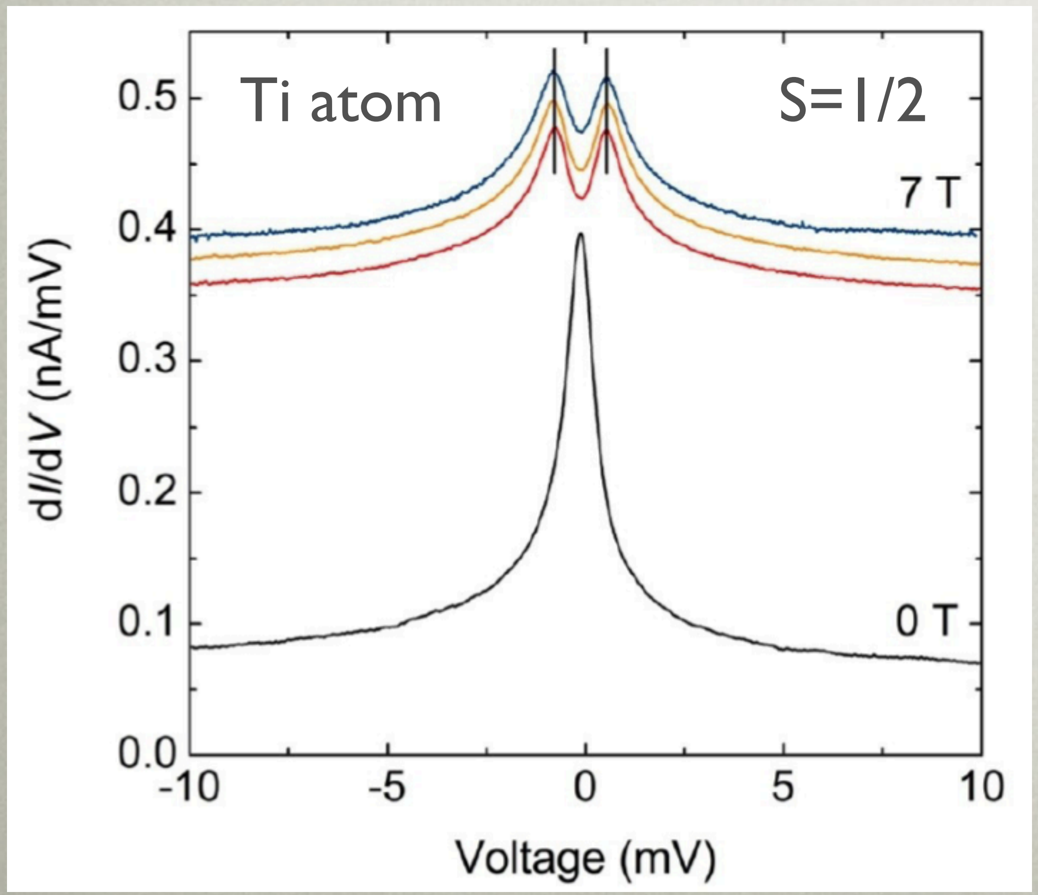
External magnetic field



Kondo resonance splitting

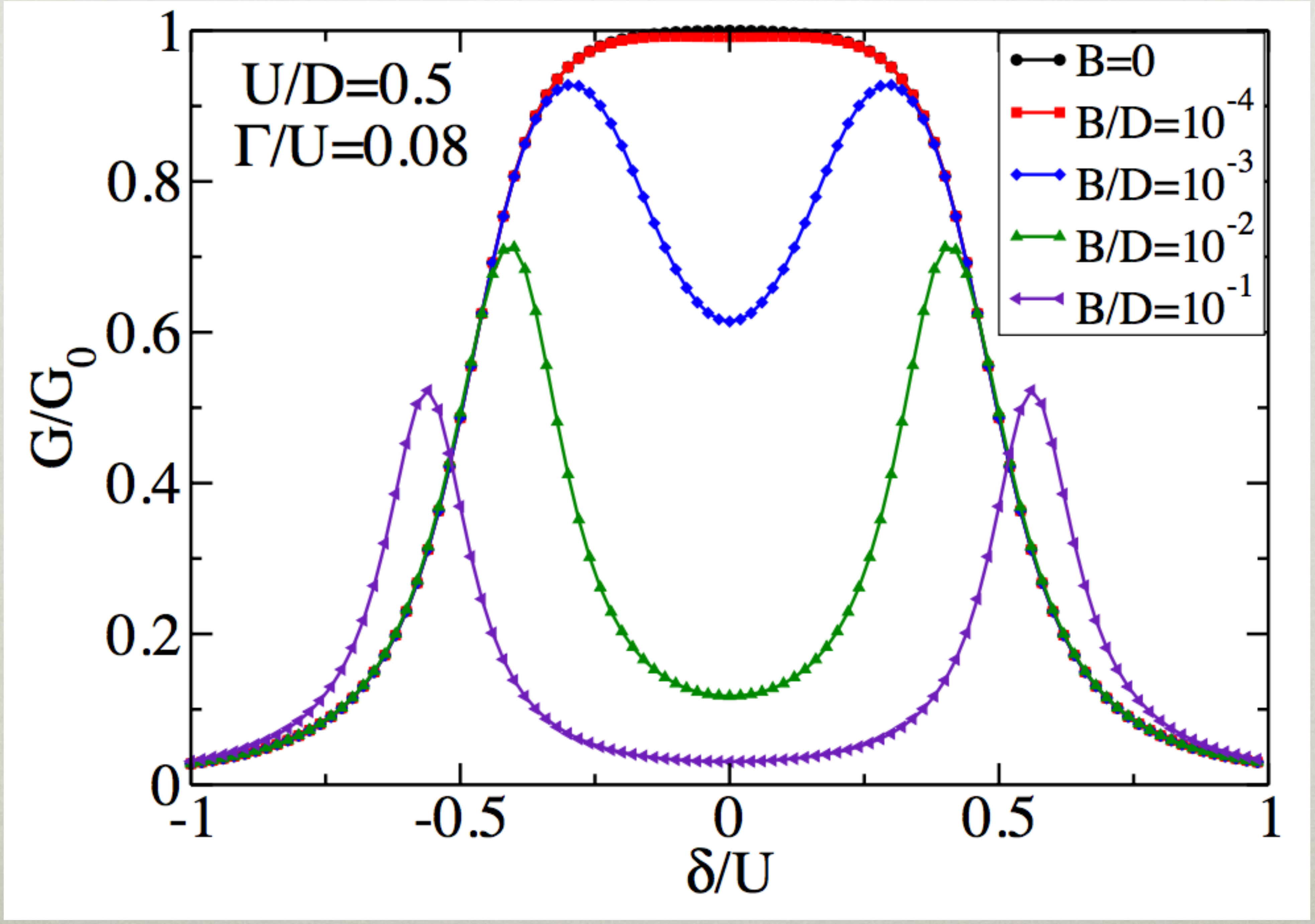






S. Otte et al., Nature Physics 4, 847 (2008)

Effect on conductance in quantum dots



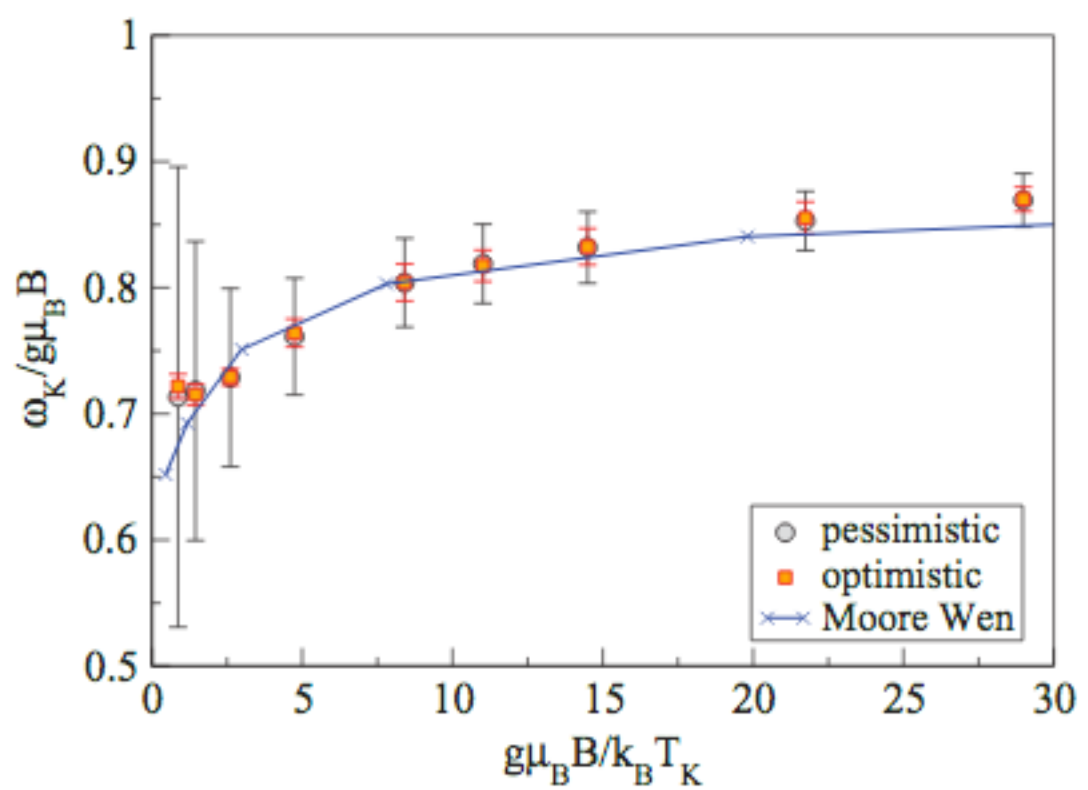
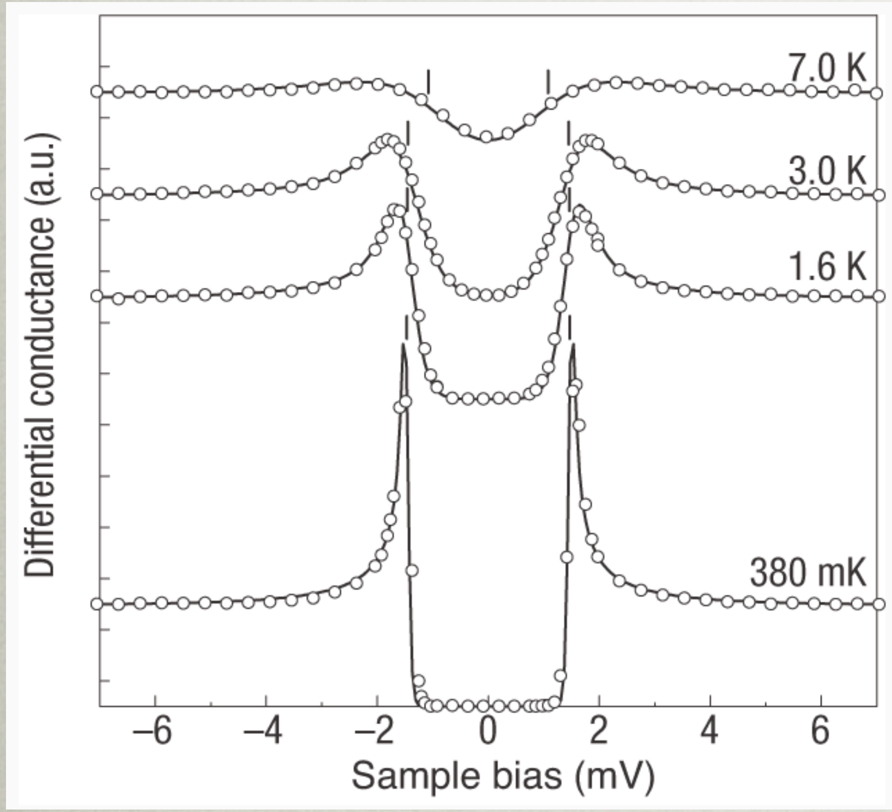
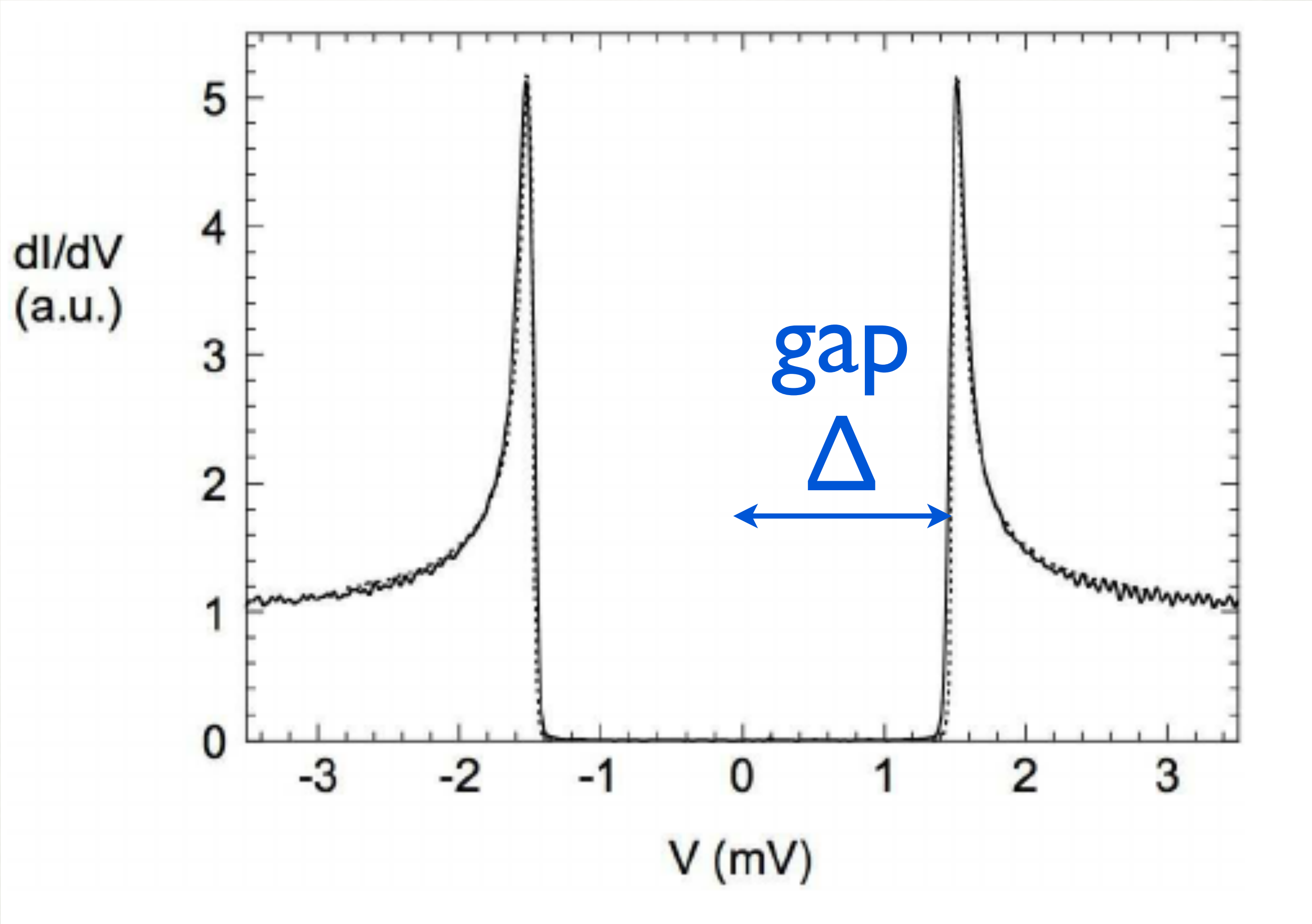


FIG. 8. (Color online) The Kondo resonance splitting as a function of the external magnetic field. The error bars correspond to the "pessimistic" and "optimistic" error estimates. Model parameters are $U = 0.1$, $\epsilon_d = -U/2$, and $\Gamma = 0.008$ in units of half-bandwidth of the (flat) conduction band. The broadening parameter is $\alpha = 0.075$. The data labeled as "Moore Wen" are taken from Fig. 2 in Ref. 37.

Superconducting gap





Nb, T=170mK, Δ=1.5meV

H. Courtois, Grenoble
PRB (2005)

scanning tunneling microscope (STM) dI/dV spectra
(proportional to the local **density of states**)

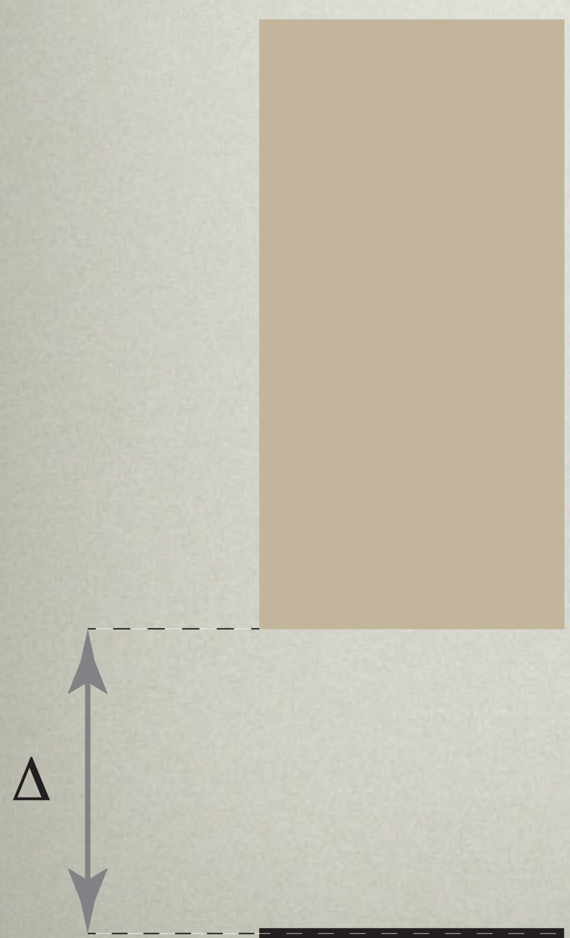
Bogoliubov quasiparticles

$$H_{\mathrm{BCS}} = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_k \Delta \left(c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} + c_{-k\downarrow} c_{k\uparrow} \right)$$

$$\gamma_{k\uparrow} = u_k c_{k\uparrow} - v_k c^\dagger_{-k\downarrow}$$

$$u_k^2 = \frac{1}{2}\left(1 + \frac{\epsilon_k}{\sqrt{\epsilon_k^2 + \Delta^2}}\right)$$

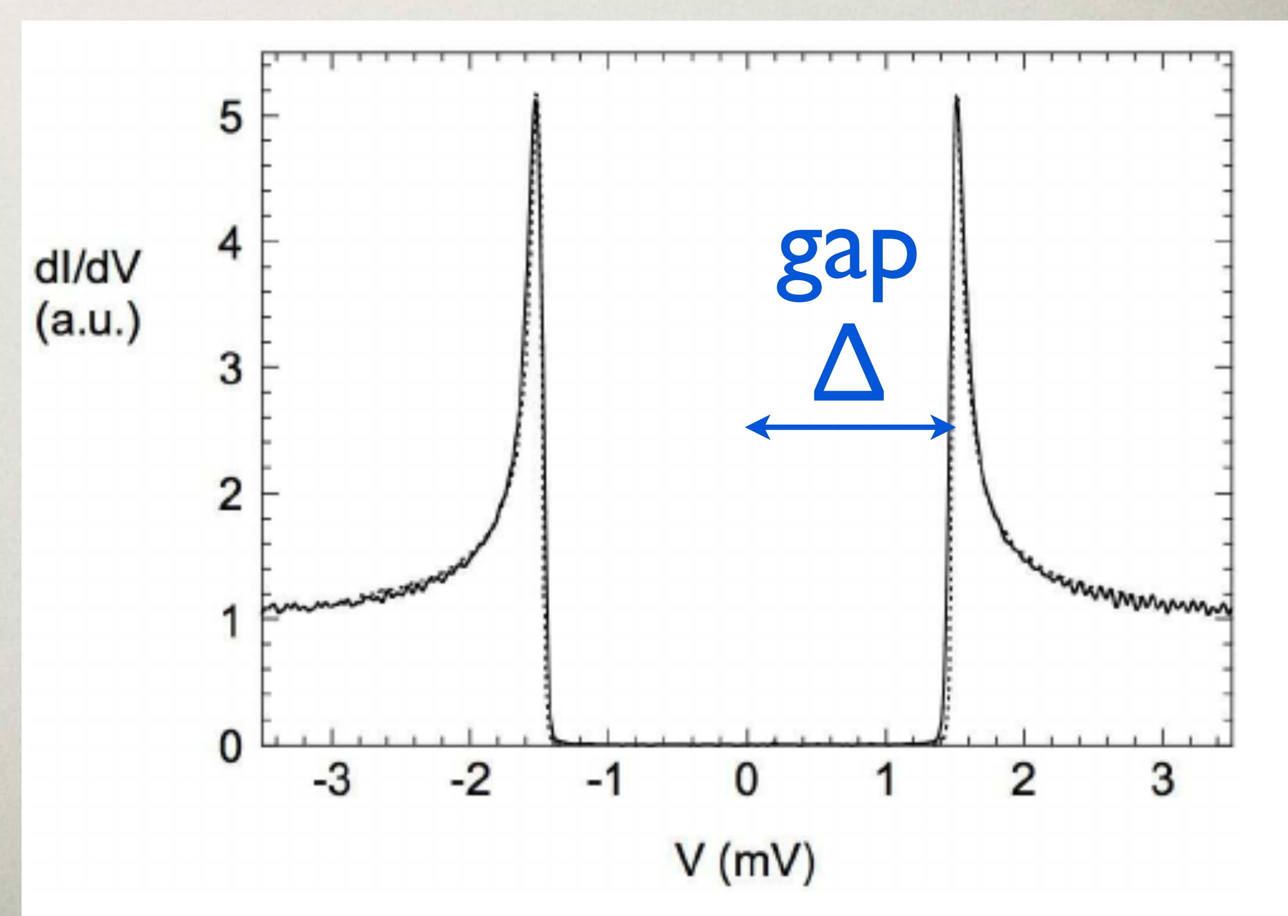
$$v_k^2 = \frac{1}{2}\left(1 - \frac{\epsilon_k}{\sqrt{\epsilon_k^2 + \Delta^2}}\right)$$



$$E_k = \sqrt{\epsilon_k^2 + \Delta^2}$$

quasiparticle continuum

ground state



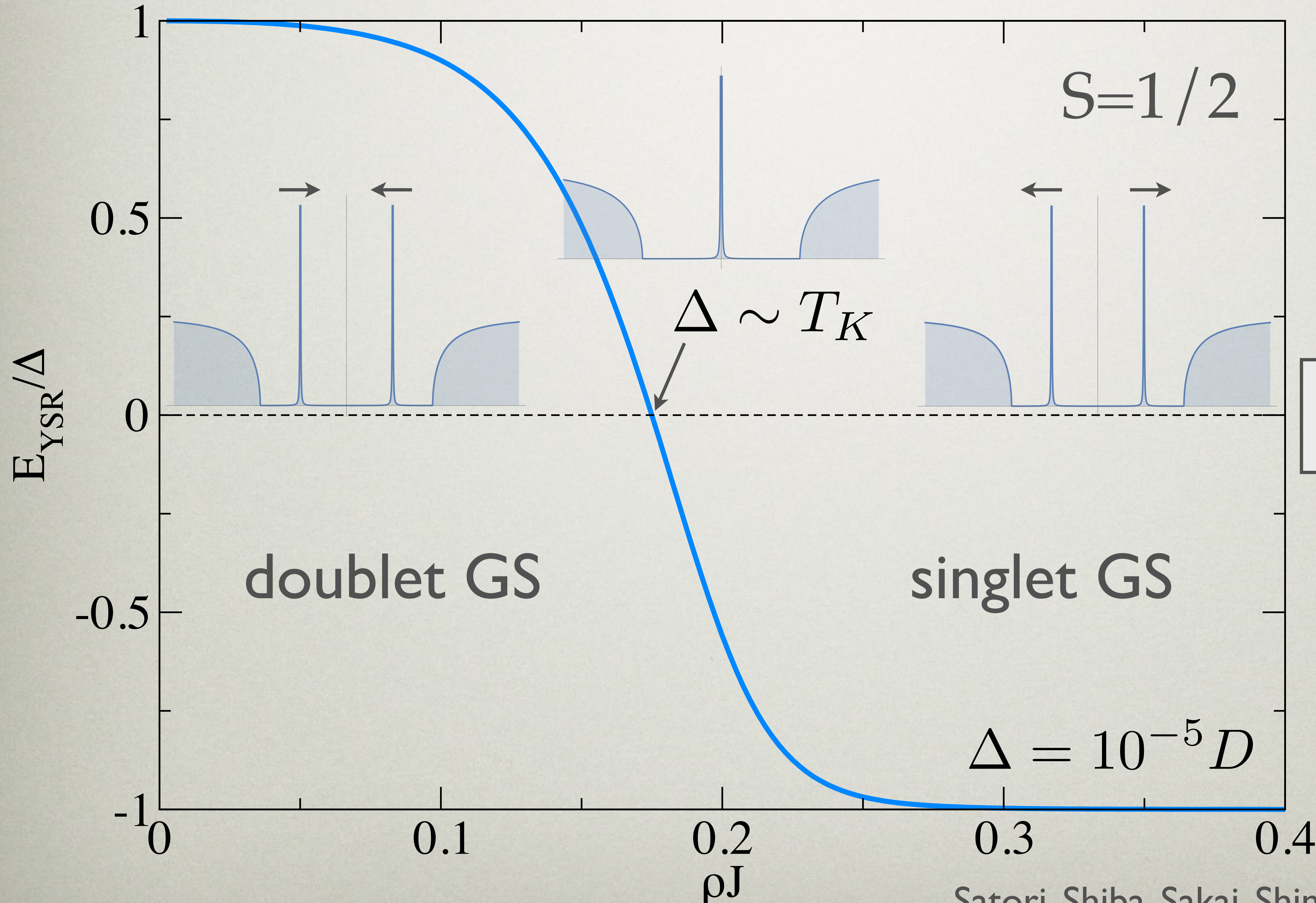
$$H_{\mathrm{BCS}} = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_k \Delta \left(c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} + c_{-k\downarrow} c_{k\uparrow} \right)$$

$$H_{\mathrm{imp}} = J\mathbf{S} \cdot \mathbf{s}(\mathbf{r} = 0)$$

$$\text{with} \quad \mathbf{s} = \frac{1}{N} \sum_{kk'} c^\dagger_k \left(\frac{1}{2} \boldsymbol{\sigma} \right) c_{k'} = f^\dagger_0 \left(\frac{1}{2} \boldsymbol{\sigma} \right) f_0$$

This is Kondo model with superconducting bath.
Difficult non-perturbative many-body problem!

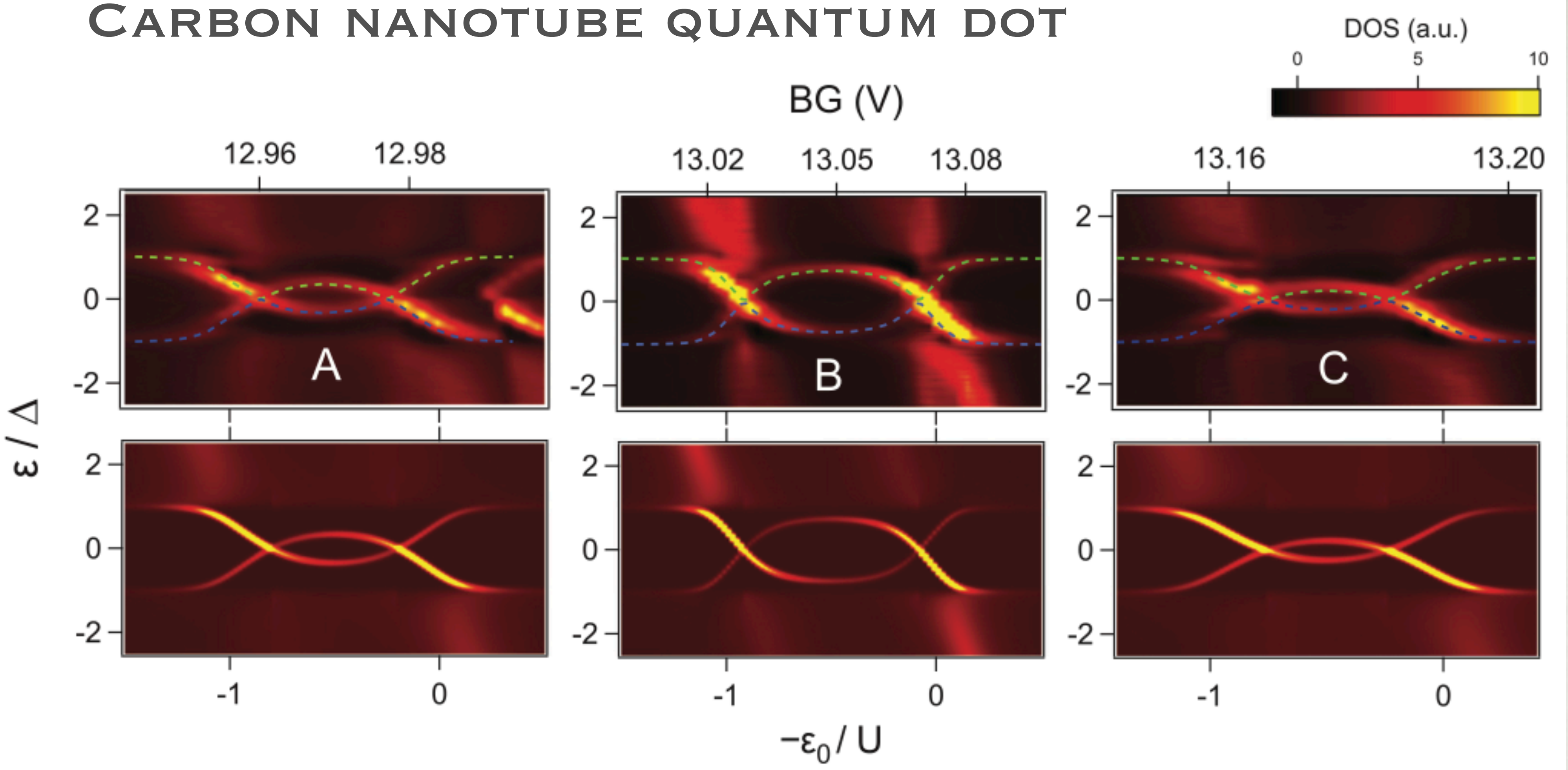
Quantum impurity in a superconductor: singlet-doublet (0-π) transition



$$T_K = \mathcal{D} \exp\left(-\frac{1}{\rho J}\right)$$

Satori, Shiba, Sakai, Shimizu JPSJ (1992);
Yoshioka, Ohashi JPSJ (1998, 2000)

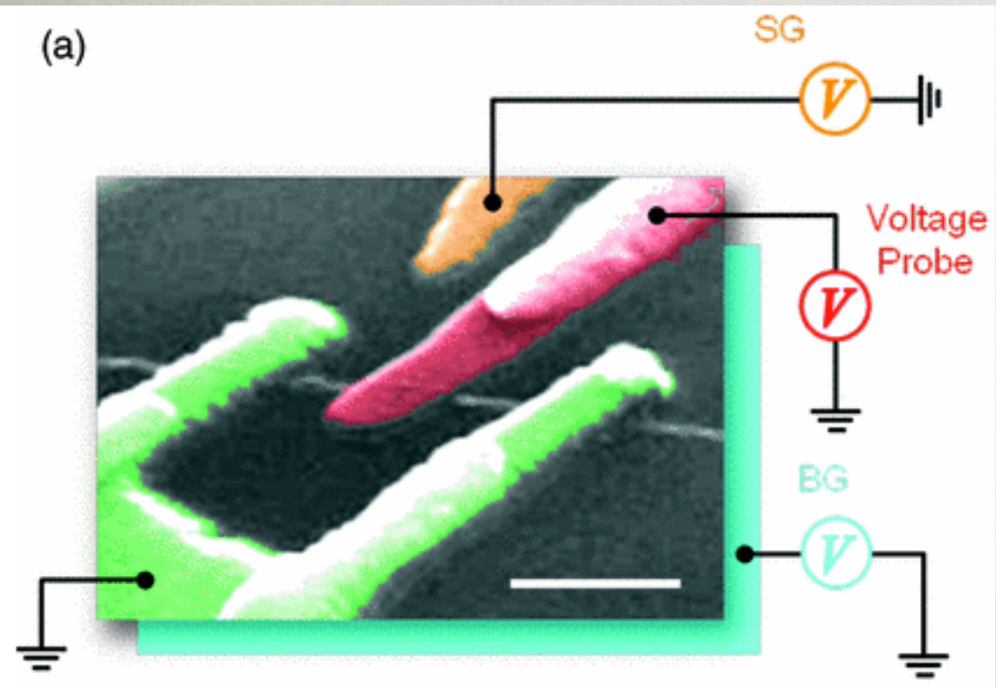
Carbon nanotube quantum dot

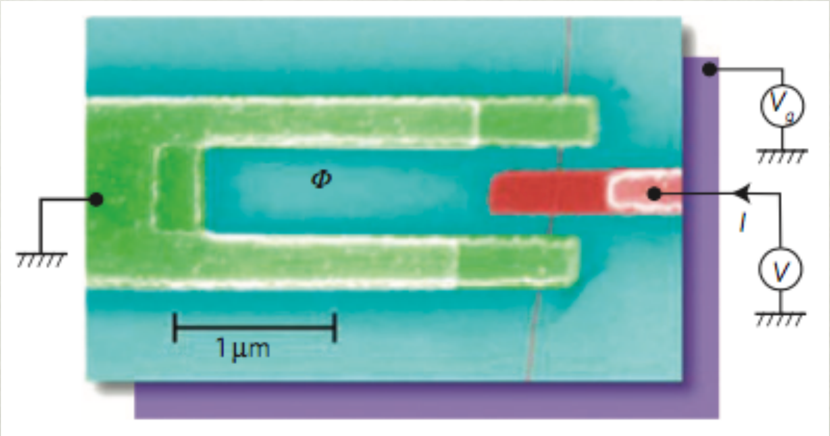


experiment

theory

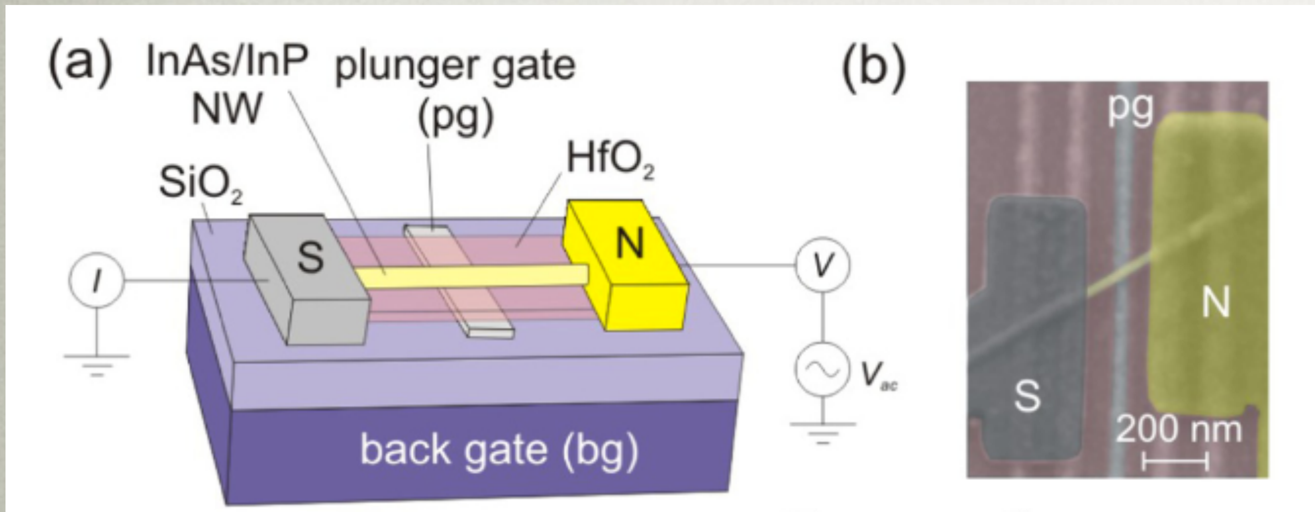
(NRG calculation)

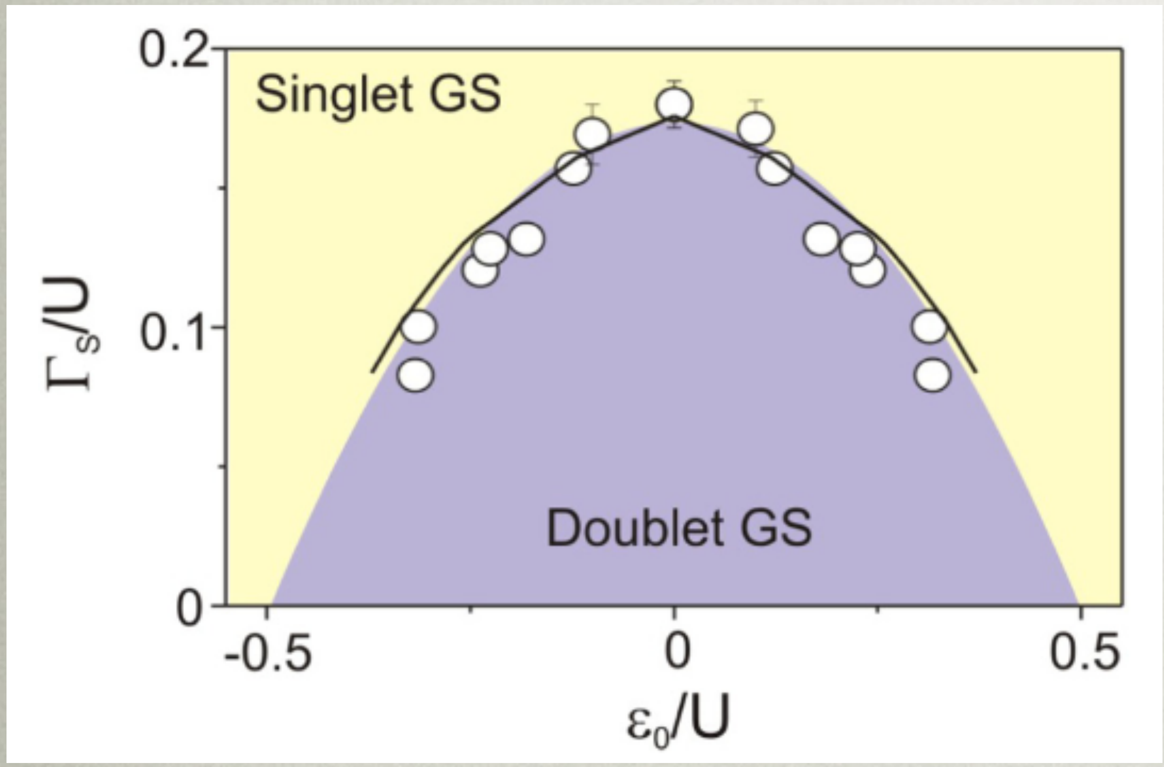


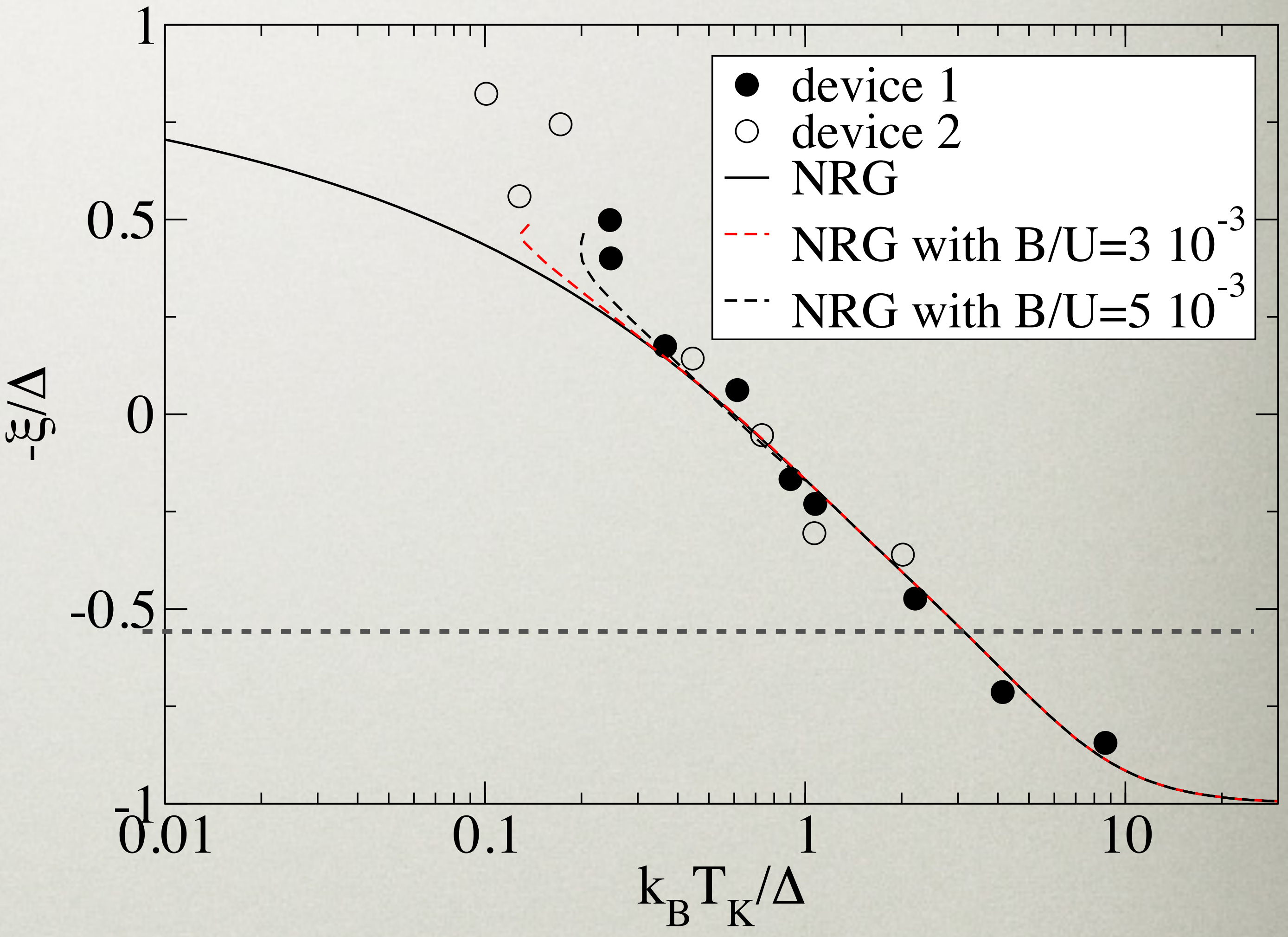


JD Pillet, P Joyez, R Žitko, MF Goffman, PRB 88, 045101 (2013)

Scaling of sub-gap excitations







Lee, Jiang, Žitko, Aguado, Lieber, de Franceschi, PRB (2017)

see also Luitz, Assaad, Novotný, Karrasch, Meden, PRL 108, 227001 (2012)