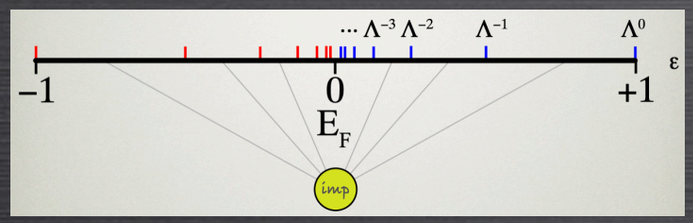
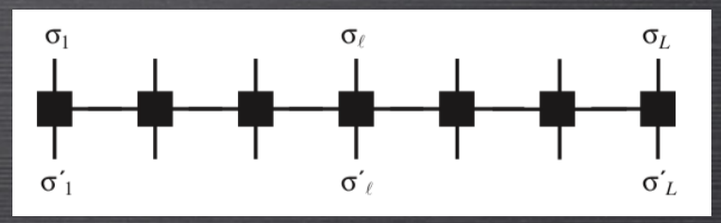
# Solvers for quantum impurity problems (with superconducting baths)

## Tutorial 4: superconducting systems





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NRG

# BCS baths in NRG

Single-channel problems:

```
bcsgap=X
```

Two-channel problems:

```
bcsgap1=X
bcsgap2=X
```

# Symmetry types

Spin SU(2) symmetry:

`symtype=SPSU2`

Spin U(1) symmetry:

`symtype=SPU1`

Fermionic parity:

`symtype=P`

No symmetry at all (super slow!):

`symtype=NONE`

Spin SU(2) symmetry & mirror symmetry:

`symtype=SPSU2LR`

Spin U(1) symmetry & mirror symmetry:

`symtype=SPU1LR`

Fermionic parity in each channel:

`symtype=PP`

# RG flow spectra

```
dumpannotated=20
dumpscaled=false
```

← Use absolute energies!

```
0 (2) [2]
0.00062594453 (1) [1]
0.001 (1) (1) (1) (1) (1) (1) (1) (1) (1) (1) (1) (1) (1) (1) (1) (1) (1) (1) (1) (3) (3) (3) (3) (3) (3) (3) (3) (3) (3) (3) (3) (3) (3) (3) (3) (3) (3) (3) (3) [80]
0.0010000021 (1) (3) [4]
```

# Spectral functions

```
broaden_max=2
broaden_min=1e-5
broaden_ratio=1.02
broaden_alpha=0.3
broaden_gamma=0.2
broaden=false
savebins=true
bins=200
```

Save raw data,
200 bins / decade

```
broaden - finite-temperature broadening tool
Usage: broaden <name> <Nz> <alpha> <T> [omega0_ratio]

Optional parameters:
 -h -- show help (when used as sole cmd line switch)
 -v -- verbose
 -m <min> -- minimal mesh frequency
 -M <max> -- maximal mesh frequency
 -r <ratio> -- ratio between two consecutive frequency points
 -o -- one .dat file
 -2 -- use the 2nd column for weight values (complex spectra)
 -3 -- use the 3rd column for weight values (complex spectra)
 -n -- normalization-conserving broadening kernel
 -s -- compute weighted integrals for testing sum-rules
 -c -- compute cumulative spectrum
 -g -- Gaussian broadening (width alpha)
 -f -- final Gaussian broadening pass
 -x -- final derFD broadening pass
 -a -- accumulation point for the mesh
 -l -- filter out low-frequency raw data
 -h -- filter out high-frequency raw data
 -P -- keep only positive input frequencies
 -N -- keep only negative input frequencies
 -A -- output only positive frequencies
 -B -- output only negative frequencies
```

# DMRG

```
params{
     parallel = true
     sc_only = true

     NBath = 100
     nref = 100
     nrange = 1

     U = 0
     epsimp = 1000
     gamma = 1e-4

     alpha = -0.4
     band_level_shift = true
     MPO = Ec

     totalSpin = true
     printTotSpinZ = true

     EnergyErrgoal = 1e-8
     overlaps = true
}

sweeps
{

sweeps
     {
     maxdim  mindim  cutoff  niter  noise
     80      20      1E-12    3     1e-3
     80      20      1E-12    3     1e-3
     80      20      1E-12    3     1e-4
     80      20      1E-12    3     1e-4
     160      1      1E-12    3     1e-6
     160      1      1E-12    3     1e-6
     160      1      1E-12    3     1e-8
     160      1      1E-12    3     1e-8
      160      1      1E-12    3     0
      320      1      1E-12    3     0
      320      1      1E-12    3     0
      320      1      1E-12    3     0
      320      1      1E-12    3     0
      320      1      1E-12    3     0
      640      1      1E-12    3     0
      640      1      1E-12    2     0
      640      1      1E-12    2     0
      640      1      1E-12    2     0
      1280     1      1E-12    2     0
      1280     1      1E-12    2     0
      1280     1      1E-12    2     0
      1280     1      1E-12    2     0
      1280     1      1E-12    2     0
      1280     1      1E-12    2     0
      2560     1      1E-12    2     0
      2560     1      1E-12    2     0
      2560     1      1E-12    2     0
      2560     1      1E-12    2     0
      2560     1      1E-12    2     0
      2560     1      1E-12    2     0
                    }
               }
```

```
params{
        parallel = true
        sc_only = true

        NBath = 10
        nref = 10
        nrange = 1

        U = 0
        epsimp = 1000
        gamma = 1e-4

        alpha = -0.4
        band_level_shift = true
        MPO = Ec

        totalSpin = true
        printTotSpinZ = true

        EnergyErrgoal = 1e-8
}
```

OpenMP parallelization over symmetry sectors (charge/spin)

don't put electrons on QD sites in initial state

N=10 energy levels in the SC island

perform calculations for n between 9 and 11

should be true

calculate spin of the states

stopping criterion for DMRG sweeps

# MPOs

**std**: dim=8, impurity at the edge
**middle**: dim=8, impurity at the center of the chain (at the Fermi level)
**Ec**: dim=9, impurity at the edge
**middle_Ec**: dim=9, impurity at the center
**Ec_V**: capacitive coupling between QD and SC island
**Ec_t**: hopping between the levels in the SC (as in Hubbard model)
**Ec_eta**: one SC level with weaker pairing interaction

**2ch**: two-channels, impurity between two SC chains
**2ch_impFirst**: two-channels, impurity at the very edge
**2ch_impFirst_V**: ... with capacitive coupling

nrsweeps=X

sweeps
{

| maxdim | mindim | cutoff | niter | noise |
|---|---|---|---|---|
| 80 | 20 | 1E-12 | 3 | 1e-3 |
| 80 | 20 | 1E-12 | 3 | 1e-3 |
| 80 | 20 | 1E-12 | 3 | 1e-3 |
| 80 | 20 | 1E-12 | 3 | 1e-4 |
| 80 | 20 | 1E-12 | 3 | 1e-4 |
| 160 | 1 | 1E-12 | 3 | 1e-6 |
| 160 | 1 | 1E-12 | 3 | 1e-6 |
| 160 | 1 | 1E-12 | 3 | 1e-8 |
| 160 | 1 | 1E-12 | 3 | 1e-8 |
| 160 | 1 | 1E-12 | 3 | 0 |
| 320 | 1 | 1E-12 | 3 | 0 |
| 320 | 1 | 1E-12 | 3 | 0 |
| 320 | 1 | 1E-12 | 3 | 0 |
| 320 | 1 | 1E-12 | 3 | 0 |
| 320 | 1 | 1E-12 | 3 | 0 |

# Magnetic field

**EZ_imp**: field on QD site

**EZ_bulk**: field on SC island

**EZx_imp**, **EZx_bulk**: fields along the x direction

# Charging term

**Ec**: charging energy

**n0**: occupancy control parameter

# Excited states

```
excited_states = 1
Weight=1000
overlaps=true
```

# Spin-orbit coupling

**lambda**: SOC strength

# Triplet states

`spin1=true`

Adds Sz=1 sectors.

# Output control

```
computeEntropy=true
chargeCorrelation=true
spinCorrelation=true
spinCorrelationMatrix=true
channelDensityMatrix=true
pairCorrelation=true
hoppingExpectation=true
calcweights=true
charge_susceptibility=true
```

# Final projects

1. Study charge-charge correlations in a QD with a superconducting bath ($\Gamma$, $\delta$, U at fixed $\Delta$).
2. Study the nature of the subgap states in SIAM as a function of $U/\Delta$ (from ABS to YSR).

3. Study the condensation energy and $\Delta'$ in the Richardson model vs. pairing strength $\alpha$. Extrapolate to large-N.
4. Try to detect the triplet counterparts to YSR singlet states. Use magnetic field to push them down into the subgap range.