Tutorial for Hierarchical Equations of Motion Approach to Quantum Impurity Systems

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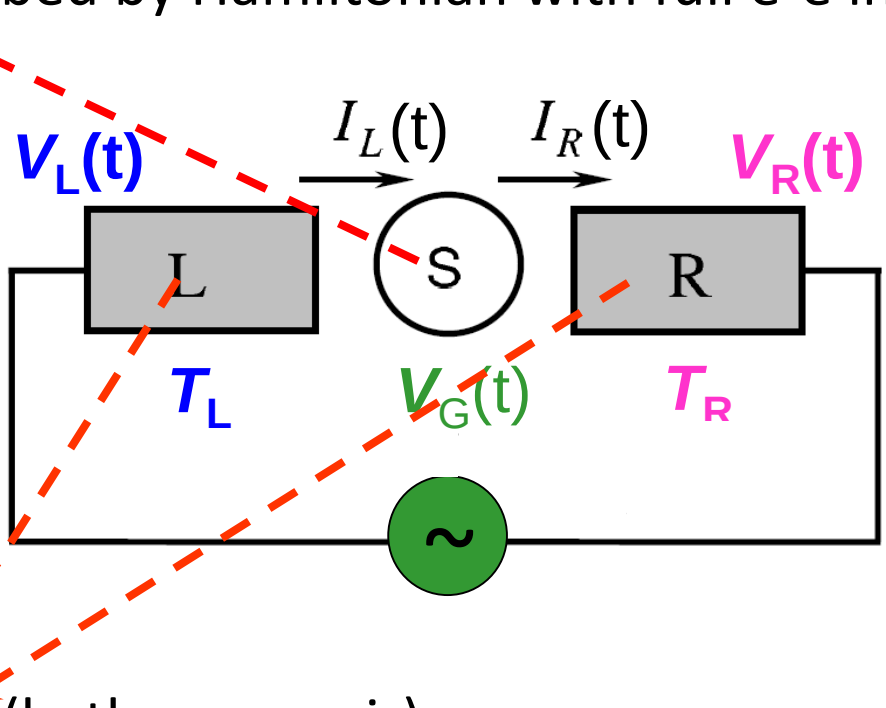
System and bath environment

System (impurity or quantum dot):

described by Hamiltonian with full e-e interactions

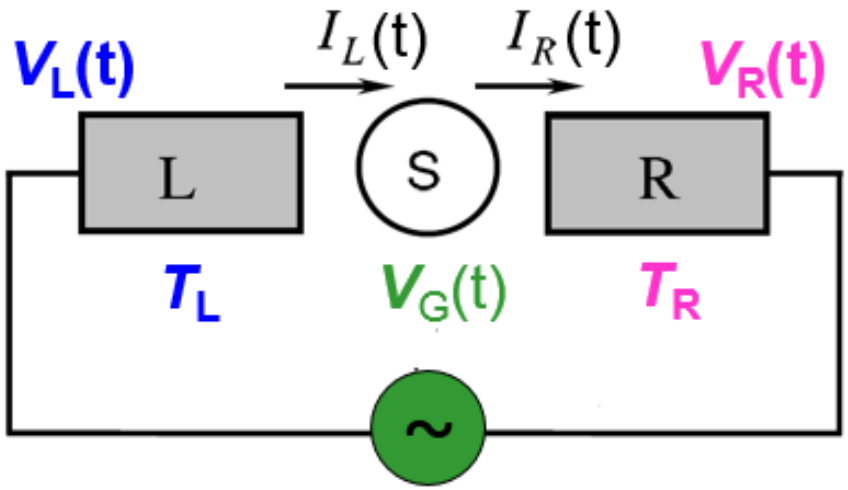


Environment (bath, reservoir):

noninteracting electrodes

play the roles of thermal bath and electron reservoir

System and bath environment



System subspace spanned by Fock states

Lead(s) characterized by spectral density function

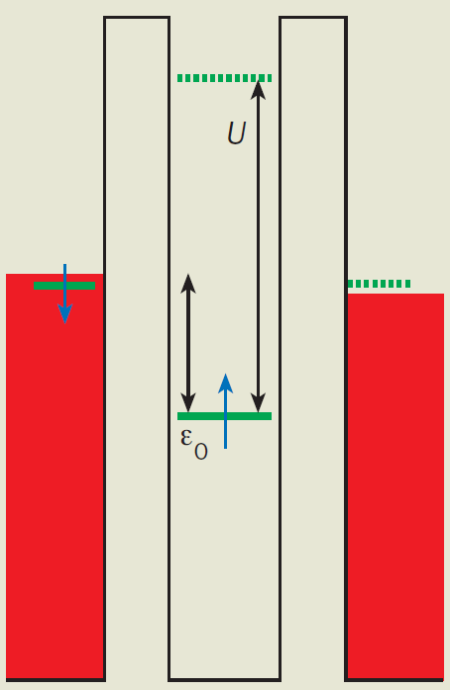
Single-level Anderson impurity model

$$H_T = H_{system} + H_{reservoir} + H_{sys-res}$$

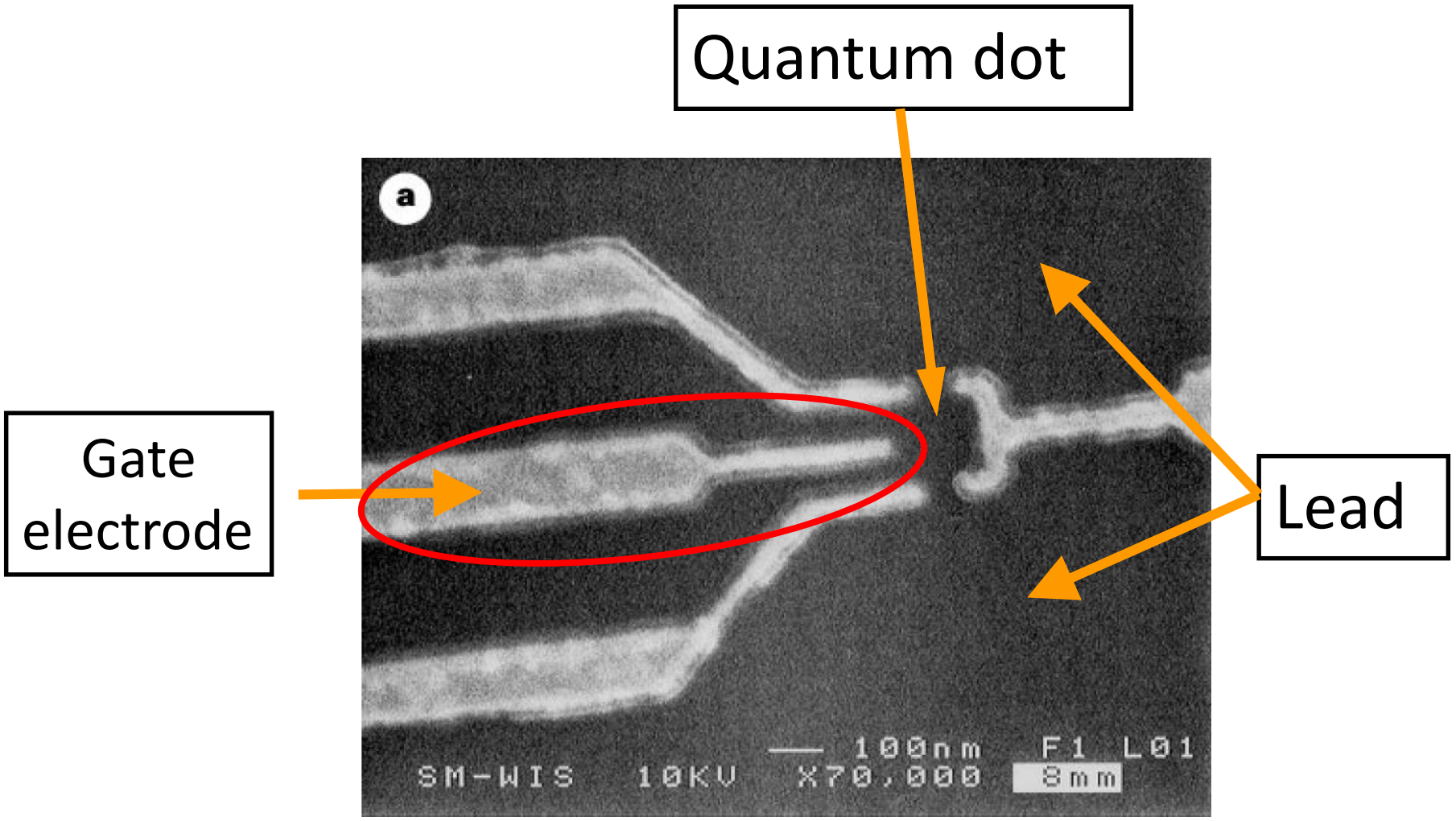
$$H_{sys} = \varepsilon_\uparrow \hat{n}_\uparrow + \varepsilon_\downarrow \hat{n}_\downarrow + U\hat{n}_\uparrow \hat{n}_\downarrow \quad \left(\hat{n}_s = a_s^+ a_s\right)$$

$$H_{res} = \sum_{\alpha=L,R} \sum_{k,s} \varepsilon_{k\alpha s} d_{k\alpha s}^+ d_{k\alpha s}$$

$$H_{sys-res} = \sum_{\alpha=L,R} \sum_{k,s} t_{k\alpha s} d_{k\alpha s}^+ a_s + \text{h.c.}$$



Kondo phenomena in quantum dots



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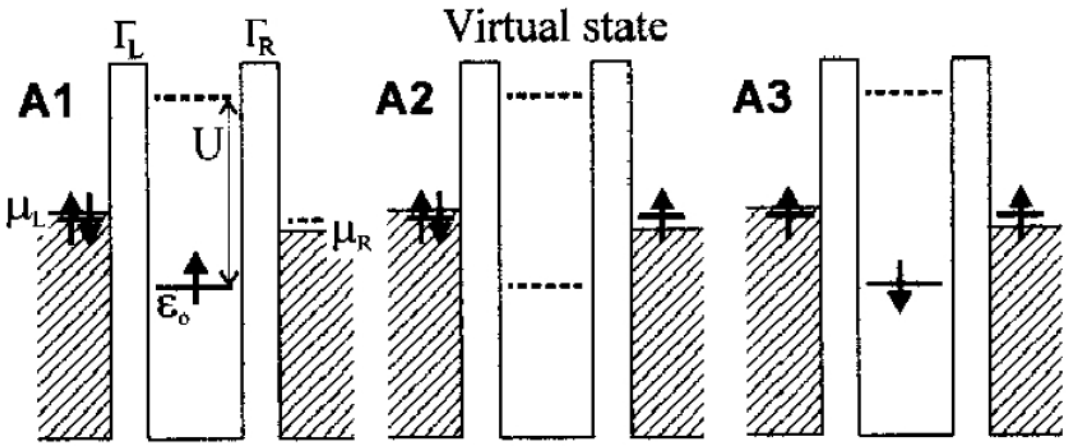
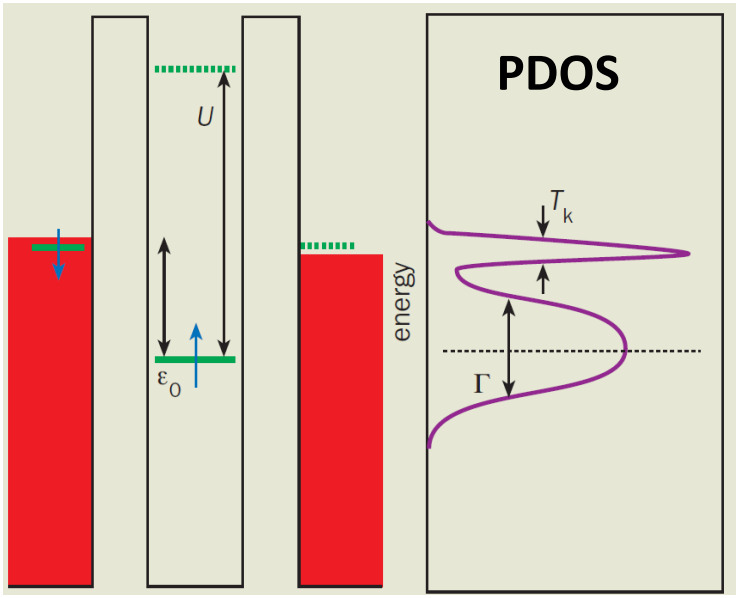


Tunneling event with an effective spin-flip (multi-electron physics)



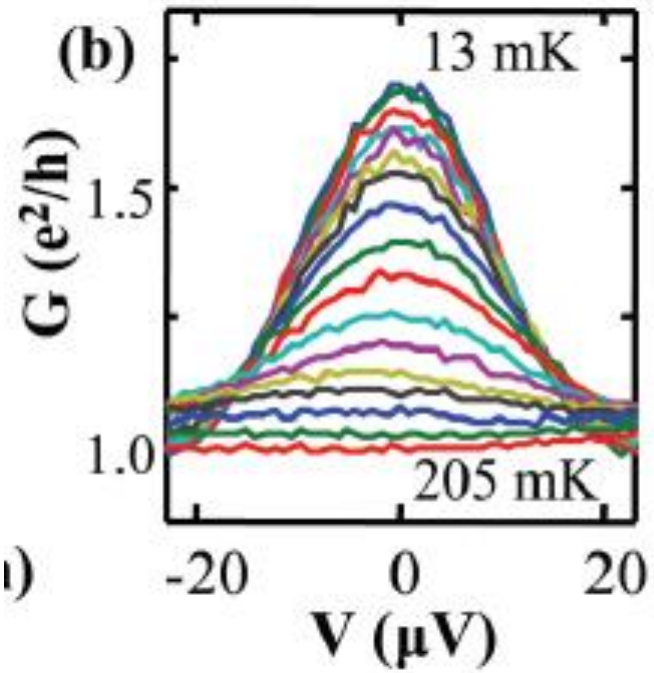
Kondo spectral peak at ε_F

Kondo, "Resistance minimum in dilute magnetic alloys", *Prog. Theor. Phys.* (1964)
Kouwenhoven and Glazman, "Revival of the Kondo effect", *Physics World* (2001)

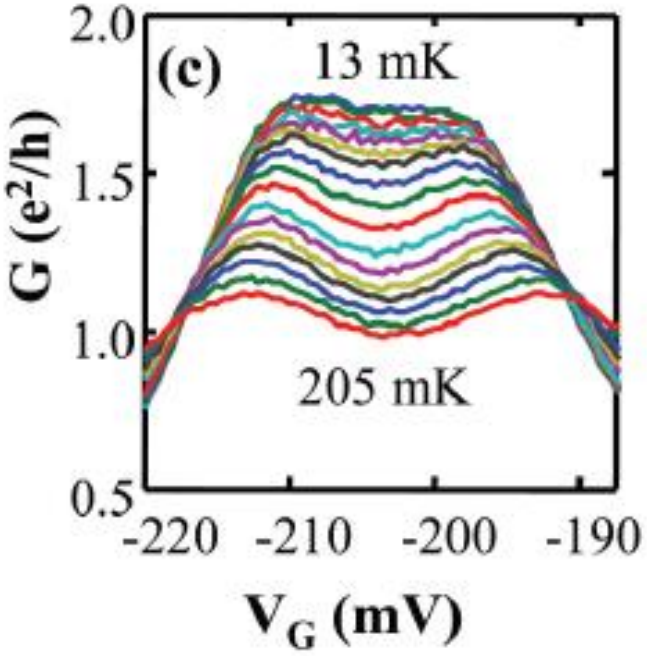
Kondo states enhance the conductance of QDs

Kondo phenomena in quantum dots

non-equilibrium conductance vs bias-voltage



equilibrium conductance vs gate-voltage (or energy level)



$G \equiv \frac{dI}{dV}$,
$V = V_L - V_R$ (or $V_R - V_L$),
V_G varies the energy level of QD

Kondo states enhance the conductance of QDs:
$T \searrow, G \nearrow$

Quantum dissipation theory

- Isolated quantum systems: Schrödinger equation

$$\dot{\rho_{\mathrm{T}}}(t) = -i\left[H_{\mathrm{T}}, \rho_{\mathrm{T}}\right]$$

- Open quantum systems: Quantum master equation

system reduced density matrix

(many-body quantity)

$$H_{\mathrm{T}} = H_{\mathrm{sys}} + H_{\mathrm{bath}} + H_{\mathrm{sb}}$$

$$\rho(t) \equiv \mathrm{tr}_{\mathrm{B}}\left[\rho_{\mathrm{T}}(t)\right]$$

dissipation superoperator

$$\dot{\rho}(t) = -i\left[H_{\mathrm{sys}}, \rho(t)\right] - \mathcal{R}\rho$$

reduced system propagator

$$\rho(t) = \mathcal{U}(t, t_0)\rho(t_0)$$

Major challenge: What is *R*, and how to evaluate?

Feynman-Vernon Path integral formalism

$$\rho(t) \equiv \mathrm{tr}_{\mathrm{B}}\rho_{\mathrm{T}}(t) \equiv \mathcal{U}(t,t_0)\rho(t_0)$$

$$\mathcal{U}(\boldsymbol{\psi},t;\boldsymbol{\psi}_0,t_0) = \int_{\boldsymbol{\psi}_0[t_0]}^{\boldsymbol{\psi}[t]} \mathcal{D}\boldsymbol{\psi}\, e^{iS[\boldsymbol{\psi}]}\mathcal{F}[\boldsymbol{\psi}]e^{-iS[\boldsymbol{\psi}']}$$

Feynman-Vernon influence functional: account for H_{sb} exclusively

Feynman and Vernon, Jr. *Annu. Phys. (N.Y.)* (1963)

Using the Gaussian statistical properties for the electrodes:

$$\mathcal{F}[\boldsymbol{\psi}] = \exp\left\{-i\int_{t_0}^{t} d\tau \mathcal{R}[\tau;\boldsymbol{\psi}]\right\}$$

dissipation functional

Jin, Zheng, and Yan *J. Chem. Phys.* (2008)

Dissipation functional and memory effect

What is the form of *R* ?

system annihilation operator in path integral formulation

$$\mathcal{R}[t;\boldsymbol{\psi}] \propto \int_{t_0}^{t} d\tau\, C_{\alpha s}(t-\tau)\, a_s[\psi(\tau)]$$

electrode correlation function (or lesser self-energy in NEGF): memory effects from system-lead couplings

How to solve for *R*? ----- *By taking its time derivative*

$$\partial_t \mathcal{R}[t;\boldsymbol{\psi}] \propto \int_{t_0}^{t} d\tau\, \partial_t C_{\alpha s}(t-\tau)\, a_s[\psi(\tau)] + C_{\alpha s}(0)\, a_s[\psi(t)]$$

Jin, Zheng, and Yan *J. Chem. Phys.* (2008)

- Decomposition of reservoir correlation function

fluctuation-dissipation theorem

$$C(t) = \int_{-\infty}^{\infty} d\omega\, e^{i\omega t}\, f_\beta(\omega)\, J(\omega) \simeq \sum_{m=1}^{M} B_m\, e^{-\gamma_m t}$$

f_b(w) – Fermi function

J(w) – reservoir spectral function (Lorentzian form)

- Existing schemes

Computation becomes more expensive as T lowers

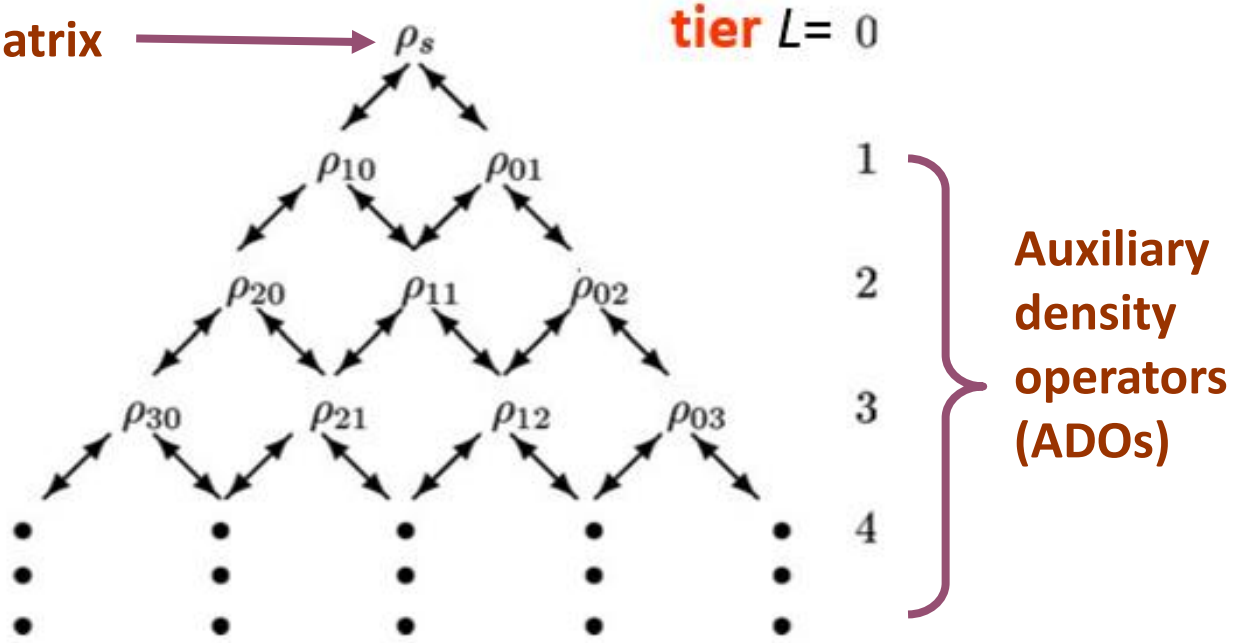
- ✓ Matsubara Spectrum Decomposition (MSD)
- ✓ MSD + Frequency Dispersion (MFD) (Zheng, Jin, and Yan et al. *JCP* 2009)
- ✓ Partial Fraction Decomposition (PFD) (Croy and Saalmann, *PRB* 2009)
- ✓ **Padé Spectrum Decomposition** (PSD) (Ozaki *PRB* 2007; Hu and Yan et al. *JCP* 2010, 2011)

Final form of HEOM

reduced system density matrix: $\rho_s(t) \equiv \rho^{(0)}(t)\mathrm{tr}_{\mathrm{res}}\rho_{\mathrm{total}}(t)$

$$\dot{\rho}^{(n)}_{j_1\cdots j_n} = -\left(i\mathcal{L} + \sum_{r=1}^{n}\gamma_{j_r}\right)\rho^{(n)}_{j_1\cdots j_n} - i\sum_{j}\mathcal{A}_{\bar{j}}\,\rho^{(n+1)}_{j_1\cdots j_n j} - i\sum_{r=1}^{n}(-)^{n-r}\,\mathcal{C}_{j_r}\,\rho^{(n-1)}_{j_1\cdots j_{r-1}j_{r+1}\cdots j_n}$$

Reduced density matrix → ρ_s



$$\bar{A} = \mathrm{Tr}(\hat{A}\rho_s)$$

➢ Model

Electrode spectral function:

electrode Hamiltonian:

$$h_{\mathrm{B}} = \sum_{\alpha} h_{\alpha} = \sum_{\alpha k} (\epsilon_{\alpha k} + \mu_{\alpha}) \hat{d}^{\dagger}_{\alpha k} \hat{d}_{\alpha k},$$

system-bath coupling:

$$H_{\mathrm{SB}} = \sum_{\alpha \mu} \left(\hat{a}^{+}_{\mu} \hat{F}^{-}_{\alpha \mu} + \hat{F}^{+}_{\alpha \mu} \hat{a}^{-}_{\mu} \right),$$

with

$$\hat{F}^{-}_{\alpha \mu} = \sum_{k} t_{\alpha \mu k} \hat{d}_{\alpha k} = (\hat{F}^{+}_{\alpha \mu})^{\dagger}.$$

bath hybridization spectral function:

$$J_{\alpha \mu \nu}(\omega) = \pi \sum\nolimits_{k} t_{\alpha \mu k} t^{*}_{\alpha \nu k} \, \delta(\omega - \epsilon_{\alpha k})$$

Lorentzian form: $$\Delta_{\alpha}(\omega) = \frac{\Delta_{\alpha} W^{2}}{(\omega - \mu_{\alpha})^{2} + W^{2}}$$

Δ_{α}: dot-lead coupling
W: band width
μ_{α}: chemical potential

➢ Model

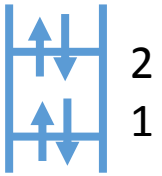
Hamiltonian of QD: Anderson model

e.g. single impurity Anderson model

$$H_{\mathrm{dot}} = \epsilon_{\uparrow} n_{\uparrow} + \epsilon_{\downarrow} n_{\downarrow} + U n_{\uparrow} n_{\downarrow} \qquad (n_{\sigma} = a_{\sigma}^{+} a_{\sigma})$$

e.g. two-level Anderson model

$$\begin{aligned} H_{\mathrm{dot}} = {} & \epsilon_{1\uparrow} n_{1\uparrow} + \epsilon_{1\downarrow} n_{1\downarrow} + \epsilon_{2\uparrow} n_{2\uparrow} + \epsilon_{2\downarrow} n_{2\downarrow} \\ & + U n_{1\uparrow} n_{1\downarrow} + U n_{2\uparrow} n_{2\downarrow} \\ & + U n_{1\uparrow} n_{2\uparrow} + U n_{1\uparrow} n_{2\downarrow} + U n_{1\downarrow} n_{2\uparrow} + U n_{1\downarrow} n_{2\downarrow} \end{aligned}$$



UserDefine model …..

see ./main/calchs.f90

Compilation

ssh to your sever

$ tar –xvf HEOM_Code
$ cd HEOM_directory

Compilation

./readme/INSTRUCTION.txt

- compiler is INTEL FORTRAN with MKL library
- OpenMP parallelization

In Makefile

NAME: define the directory where the complied HEOM executable file will appear;
e.g. NAME=/home/home/aa/heom

LIBDIR: where is your Fortran and MKL library?

```
>make clean
```

delete objects/*.o objmod/*.mod

```
>make
```

obtain the HEOM executable file; can be of any name, e.g. heom

Compilation

```
ifort -openmp -O2 -module objmod -c module/auxmod.f90
update module/auxmod
ifort -openmp -O2 -module objmod -c module/auxmod_omp.f90
update module/auxmod_omp
ifort -openmp -O2 -module objmod -c module/bicgmod.f90
update module/bicgmod
ifort -openmp -O2 -module objmod -c module/bicgmod_omp.f90
update module/bicgmod_omp
ifort -openmp -O2 -module objmod -c module/corrfuncmod.f90
update module/corrfuncmod
```

……

Compiling ----/public/home/test/lzye/HEOM/work/heom-- done !

Steady state

Sample input file for single-level QD

```
   2      for steady/equilibrium  states
   3      # of truncation tiers=3, i.e. L = 2 (0, 1, 2)
  08      # of pade poles
   1      # energy level
   2      # of spin, 1 for spinless, 2 for spin-up and down
   2      # of leads
 0.300000E+001    0.300000E+001      band width W, (W_L, W_R)
 0.100000E+000    0.100000E+000      dot-lead coupling Δ, (Δ_L, Δ_R)
 0.200000E-001    0.200000E-001      temperature T, (T_L, T_R)
 0.1   0.1   -0.1   -0.1             energyshift/bias voltage V, (V_L↑, V_L↓, V_R↑, V_R↓)
 0.100000E+004                      time evolution length (not used for steady state)
 0.200000E-001                      time step (not used for steady state)

$para1  eup=   -0.750000  edown=   -0.750000  uu=    1.500000  fixdot=T  $end

$field  fieldtype= 0  $end
 0.100000E-019    0.100000E-019    0.100000E-019    0.100000E-019

 $jobinfo lsparse=T  $end  $end   sparse mode
```

these parameters are explained in next page

```
$para1  eup=   -0.750000  edown=   -0.750000  uu=    1.500000  fixdot=T  $end
```

parameters for dot Hamiltonian

$$H_{\mathrm{dot}} = \epsilon_{\uparrow} n_{\uparrow} + \epsilon_{\downarrow} n_{\downarrow} + U n_{\uparrow} n_{\downarrow} \qquad (n_{\sigma} = a_{\sigma}^{+} a_{\sigma})$$

fixdot = T : the Hamiltonian is not affected by the applied bias voltage

characteristic time, tchar

```
$field  fieldtype= 0  $end
 0.100000E-019    0.100000E-019    0.100000E-019    0.100000E-019
```

fieldtype = 0: exponential voltage

$$V(t) = V * \left[1 - \exp\left(-\frac{t}{\mathrm{tchar}}\right)\right]$$

fieldtype = 1: sinusoidal voltage

$$V(t) = V * \sin\left[2 * \pi * \frac{t}{\mathrm{tchar}}\right]$$

fieldtype = -1: delta-type voltage

$$V(t) = V * \delta(t = 0)$$

fieldtype = define your own fiedltype

/main/getengyshift.f90

Construct system subspace in a Fock-state basis set

e.g. single impurity Anderson model

$$H_{\mathrm{dot}} = \epsilon_{\uparrow} n_{\uparrow} + \epsilon_{\downarrow} n_{\downarrow} + U n_{\uparrow} n_{\downarrow} \qquad (n_s = a_s^{+} a_s)$$

empty $|0\rangle$, single occu. $|\uparrow\rangle$ or $|\downarrow\rangle$, double occu. $|2\rangle$

anti-commutation properties!

$$a_{\uparrow} = |0\rangle\langle\uparrow| + |\downarrow\rangle\langle 2| \quad \Big\} \quad a_{\uparrow}^{+}$$
$$a_{\downarrow} = |0\rangle\langle\downarrow| - |\uparrow\rangle\langle 2| \quad \Big\} \quad a_{\downarrow}^{+} \quad ?$$

matrix representation :

$$\begin{array}{c} \\ |0\rangle \\ |\uparrow\rangle \\ |\downarrow\rangle \\ |2\rangle \end{array} \begin{array}{c} \langle 0| \ \langle\uparrow| \ \langle\downarrow| \ \langle 2| \\ \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix} \end{array} = a_{\uparrow}$$

$$a_{\downarrow} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

occupation: $N_\uparrow = \mathrm{Tr}(n_\uparrow \rho_s) = \rho_{22} + \rho_{44}$

$N_\downarrow = \mathrm{Tr}(n_\downarrow \rho_s) = \rho_{33} + \rho_{44}$

run the HEOM:

```
./heom < input > out
```

output file:

```
occupation, spin up =   0.499999999974057
              down =    0.499999999973872
             jleft  =     791.046564390890        pA
            jright  =    -791.046556404541        pA

spin current
             jleftu =     395.523282195495        pA
             jleftd =     395.523282195395        pA
            jrightu =    -395.523278201808        pA
            jrightd =    -395.523278202733        pA
```

$$I_\alpha(t) = -2\,\mathrm{Im}\sum_{j\in\alpha}\mathrm{tr}\left[\hat{a}_\mu\,\rho_j^{(1)}(t)\right]$$

electric current:

$$I_L + I_R = 0$$

$$I_L = I_{L\uparrow} + I_{L\downarrow}$$

$$I_R = I_{R\uparrow} + I_{R\downarrow}$$

reduced system density matrix ρ_s :

real part

	1	2	3	4
1	0.328442D-01	0.000000D+00	0.000000D+00	0.000000D+00
2	0.000000D+00	0.467156D+00	0.000000D+00	0.000000D+00
3	0.000000D+00	0.000000D+00	0.467156D+00	0.000000D+00
4	0.000000D+00	0.000000D+00	0.000000D+00	0.328442D-01

imag part

	1	2	3	4
1	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
2	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
3	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00
4	0.000000D+00	0.000000D+00	0.000000D+00	0.000000D+00

$$N_{\uparrow} = \mathrm{Tr}(n_{\uparrow}\rho_s) = \rho_{22} + \rho_{44}$$

$$N_{\downarrow} = \mathrm{Tr}(n_{\downarrow}\rho_s) = \rho_{33} + \rho_{44}$$

check ρ_s:

👍 rho is found OK!

👎 checkrho: Warning! rho is not positive definite!

time used:

```
SJ_DBG_TIMER_STOP : ntimer=   1 CPU=[        2.43215] REAL= [        1.22659]
```

memory used:

```
    general memory cost estimated   0.208854675292969       MB
        rk4 memory cost estimated   0.000000000000000E+000  MB
       bicg memory cost estimated   0.000000000000000E+000  MB
       diis memory cost estimated   0.000000000000000E+000  MB
      tfqmr memory cost estimated   0.366394042968750       MB
    corrfun memory cost estimated   0.000000000000000E+000  MB
```

Total memory used = general memory + tfqmr memory

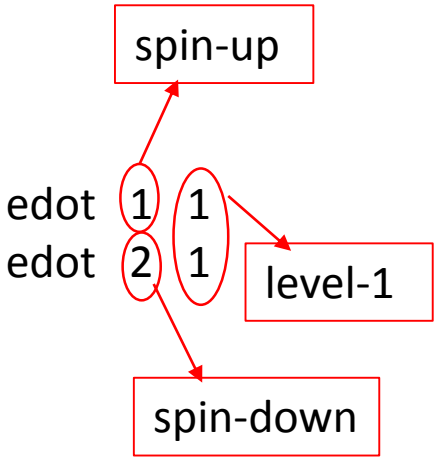
```
     Total memory used        0.575248718261719       MB
```

```
    2
    3
   08
    1
    2
    2
 0.300000E+001    0.300000E+001
 0.100000E+000    0.100000E+000
 0.200000E-001    0.200000E-001
 0.1   0.1   -0.1   -0.1
 0.100000E+004
 0.200000E-001

 $hamil_sys  lgenhs=.true.$end
 hsys
 edot  1  1        -1.50
 edot  2  1        -1.50
 udot  0  1         1.50

 $field  fieldtype= 0  $end
  0.100000E-019    0.100000E-019    0.100000E-019    0.100000E-019

 $jobinfo lsparse=T  $end
```



main/genhs.f90

eup – 0.5*udot
edown – 0.5*udot

convergence test

truncation level L

# of pade poles M

if $T \searrow$, then $L \nearrow$ and $M \nearrow$

quantities: current I, spectral function $A(\omega)$, occupation N …

test with:

$$L \quad \text{vs.} \quad L+1$$
$$M \quad \text{vs.} \quad M+1$$

convergence test

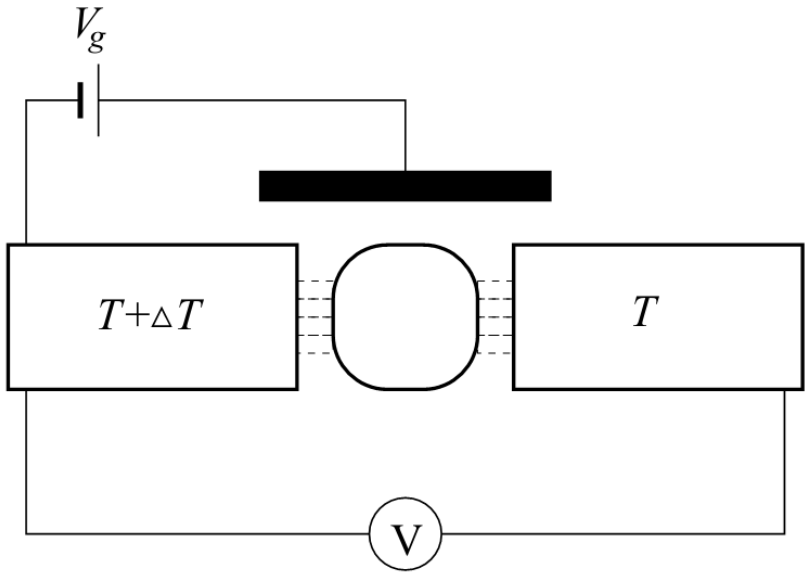
Equilibrium electron occupation on quantum dot

L	# of unknowns	Memory (Mbytes)	CPU time (seconds)	$\langle n_s \rangle$ (s = ↑or↓)
1	**112**	**0.1**	**1.1**	**0.50003**
2	**3,492**	**0.4**	**1.3**	**0.49174**
3	**30,532**	**5.9**	**5.3**	**0.47842**
4	**514,548**	**106.3**	**84.4**	**0.48235**
5	**3,306,428**	**1261.0**	**867.2**	**0.48226**
6	**38,914,728**	**17057.6**	**10156.8**	**0.48227**

Error less than 0.0001 at $L = 4$ — deemed as converged

Example: steady state calculations

- Thermopower in Kondo QDs



direction of electron flow?

Thermopower (Seeback coefficient)

$$S_{\mathrm{def}} \equiv -\left(\frac{V_T}{\Delta T}\right)_{I=0} = \left(\frac{V}{\Delta T}\right)_{I=0}$$

ΔT: temperature difference

V_T: thermovoltage

V: the voltage that cancels exactly the current induced by ΔT

Sign of S – direction of electron flow under temperature gradient

Example: steady state calculations

➢ Thermopower in Kondo QDs

In linear response regime:

total electric current:

$$I = GV + L_T \Delta T$$

transport coefficients:

$$G = \left(\frac{\partial I}{\partial V}\right)_{\Delta T=0} \qquad L_T = \left(\frac{\partial I}{\partial \Delta T}\right)_{V=0}$$

G: conductance

$$S_{\text{linear}} = -L_T/G.$$

How to calculate G and L_T ??

Example: steady state calculations

➢ Calculation of conductance G

$$G = \left(\frac{\partial I}{\partial V}\right)_{\Delta T=0}$$

finite difference method:

under a bias-voltage $V = V_L - V_R$:

$$G = \frac{\Delta I}{\Delta V} = \frac{I' - I''}{V' - V''}$$

ΔV is very small (linear response), e.g. $\Delta V = 0.001$

$$V' = V + 0.5 * \Delta V$$
$$V'' = V - 0.5 * \Delta V$$

bias-voltage is antisymmetrically applied to the QD:
the input file in Page 17, line 10:
0.5*V, 0.5*V, -0.5*V, -0.5*V

Example: steady state calculations

➢ Calculation of conductance G

$$V' = V + 0.5 * \Delta V$$
$$V'' = V - 0.5 * \Delta V$$

1) set the voltage as

$0.5 * V$', $0.5 * V$', $-0.5 * V$', $-0.5 * V$'

then I' is obtained

2) set the voltage as

$0.5 * V''$, $0.5 * V''$, $-0.5 * V''$, $-0.5 * V''$

then I'' is obtained

finally, G is calculated as

$$G = \frac{\Delta I}{\Delta V} = \frac{I' - I''}{V' - V''}$$

- specially, the equilibrium (i.e. zero-bias, $V = 0$) G can be calculated as

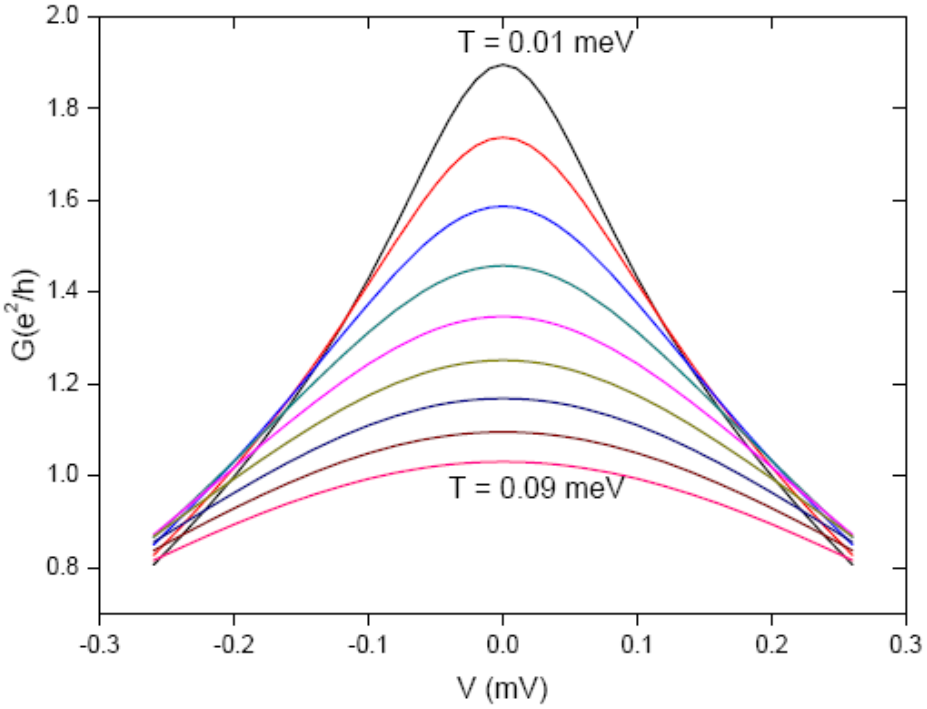
$0.5 * \Delta V$, $0.5 * \Delta V$, $-0.5 * \Delta V$, $-0.5 * \Delta V$

→ I → $G = \frac{I}{\Delta V}$

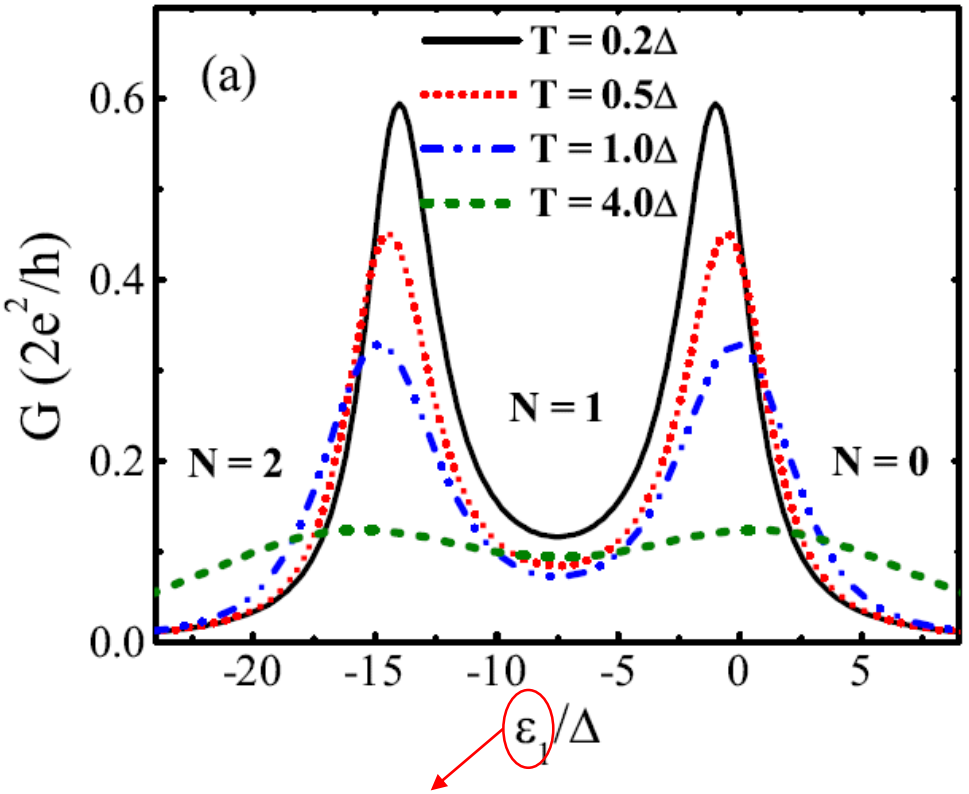
convergence test! and then

➢ Calculation of conductance G

nonequilibrium G vs V



equilibrium G vs energy level $\epsilon_\uparrow = \epsilon_\downarrow$



by varying the following eup and edown

```
$para1  eup=   -0.750000  edown=   -0.750000  uu=    1.500000  fixdot=T  $end
```

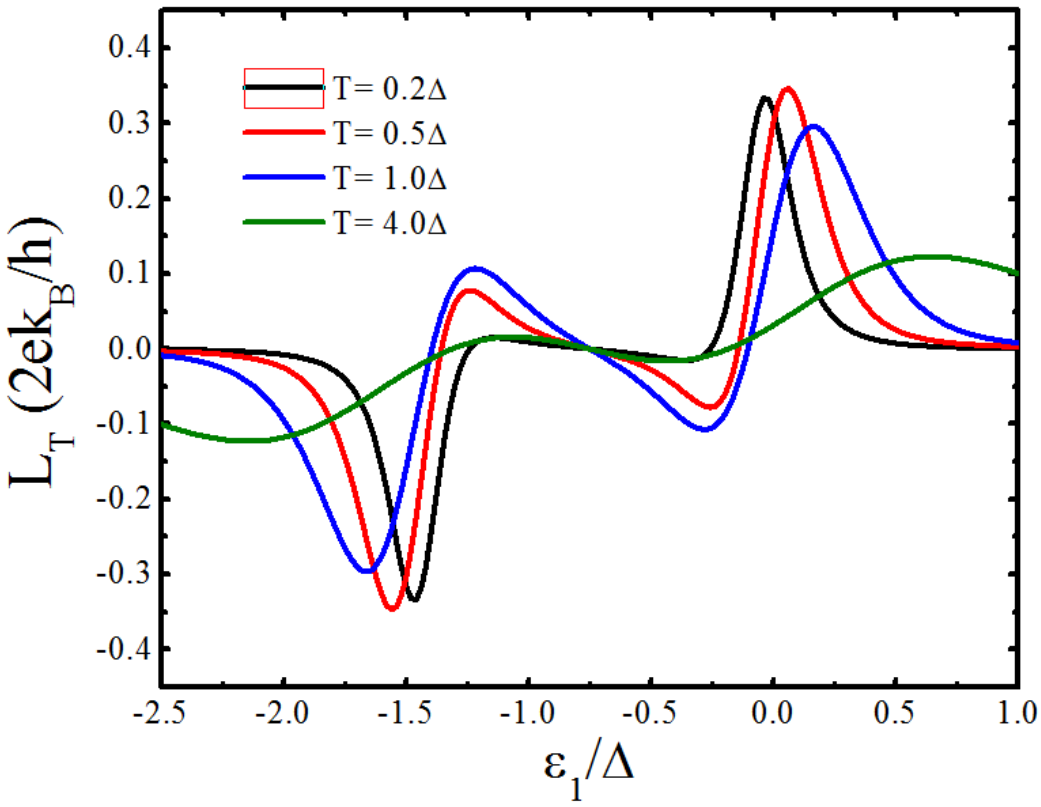
➢ Calculation of L_T

$$L_T = \left(\frac{\partial I}{\partial \Delta T}\right)_{V=0}$$

at equilibrium,
set the temperature as

$T + 0.5 * \Delta T$, $T - 0.5 * \Delta T$

$\Rightarrow$ I $\Rightarrow$ $L_T = \dfrac{I}{\Delta T}$



Two-level QDs

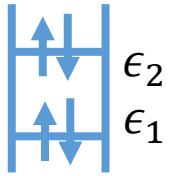
➢ Model

two-level Anderson model

$$H_{\mathrm{dot}} = \epsilon_{1\uparrow} n_{1\uparrow} + \epsilon_{1\downarrow} n_{1\downarrow} + \epsilon_{2\uparrow} n_{2\uparrow} + \epsilon_{2\downarrow} n_{2\downarrow}$$
$$+ U n_{1\uparrow} n_{1\downarrow} + U n_{2\uparrow} n_{2\downarrow}$$
$$+ U n_{1\uparrow} n_{2\uparrow} + U n_{1\uparrow} n_{2\downarrow} + U n_{1\downarrow} n_{2\uparrow} + U n_{1\downarrow} n_{2\downarrow}$$

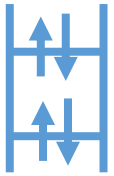
$$\delta\epsilon = \epsilon_2 - \epsilon_1$$

intra-level Coulomb energy



inter-level Coulomb energy

Sample input file for two-level QDs



```
    2      for steady/equilibrium  states
    5      # of truncation tiers=5, i.e. L = 4 (0, 1, 2, 3, 4)
   12      # of pade poles
    2      # energy level
    2      # of spin, 1 for spinless, 2 for spin-up and down
    2      # of leads
 0.800000E+001    0.800000E+001    band width W, (W_L, W_R)
 0.100000E+000    0.100000E+000    0.100000E+000    0.100000E+000
 0.505000E-001    0.495000E-001    temperature T, (T_L, T_R)
 0.000000E+000    0.000000E+000    0.000000E+000    0.000000E+000
 0.100000E+004    time evolution length (not used for steady state)
 0.200000E-001    time step (not used for steady state)
```

dot-lead coupling Δ, $(\Delta_{L1}, \Delta_{L2}, \Delta_{R1}, \Delta_{R2})$

amplitude of bias voltage V, $(V_{L\uparrow}, V_{L\downarrow}, V_{R\uparrow}, V_{R\downarrow})$

```
$hamil_sys  lgenhs=.true.$end
hsys
edot  1  1     -0.7000
edot  2  1     -0.7000
edot  1  2     -0.6000
edot  2  2     -0.6000
udot  0  1      2.0000
udot  0  2      2.0000
ucoup  0  2  1      2.0000

$field  fieldtype= 0  $end
 0.100000E-019    0.100000E-019    0.100000E-019    0.100000E-019

$jobinfo lsparse=T  $end
```

sparse mode

```
$hamil_sys  lgenhs=.true.$end
hsys
edot   1   1      -0.7000
edot   2   1      -0.7000
edot   1   2      -0.6000
edot   2   2      -0.6000
udot   0   1       2.0000
udot   0   2       2.0000
ucoup   0   2   1       2.0000
```

$\leftarrow \epsilon_{1\uparrow} - 0.5 * U_1$

$\leftarrow \epsilon_{1\downarrow} - 0.5 * U_1$

$\leftarrow \epsilon_{2\uparrow} - 0.5 * U_2$

$\leftarrow \epsilon_{2\downarrow} - 0.5 * U_2$

or equivalently,

```
$para4
e1up=0.3d0
e1down=0.3d0
e2up=0.4d0
e2down=0.4d0
u12=2.d0
uu1=2.d0
uu2=2.d0  $end
```

edot 1 1 → spin-up, level-1: $\epsilon_{1\uparrow} - 0.5 * U_1$

edot 2 1 → spin-down, level-1

edot 1 2 → spin-up, level-2: $\epsilon_{2\uparrow} - 0.5 * U_2$

edot 2 2 → spin-down, level-2

udot 0 1 → intra-level U_1 for level-1

udot 0 2 → intra-level U_2 for level-2

ucoup 0 2 1 → inter-level U_{12} between level-1 and level-2

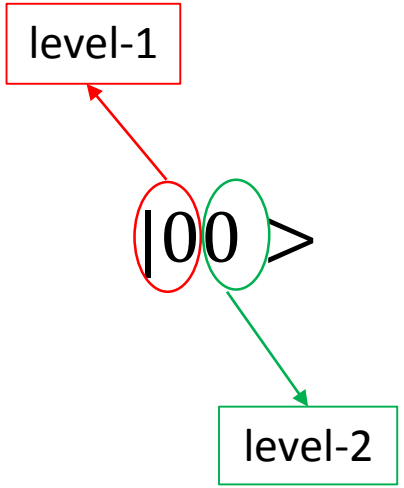
Output file

```
real part of equilibrium Hamiltonian
```

dimension of Hamiltonian: 16×16

from 1 to 16, they are $(u = \uparrow, d = \downarrow)$:

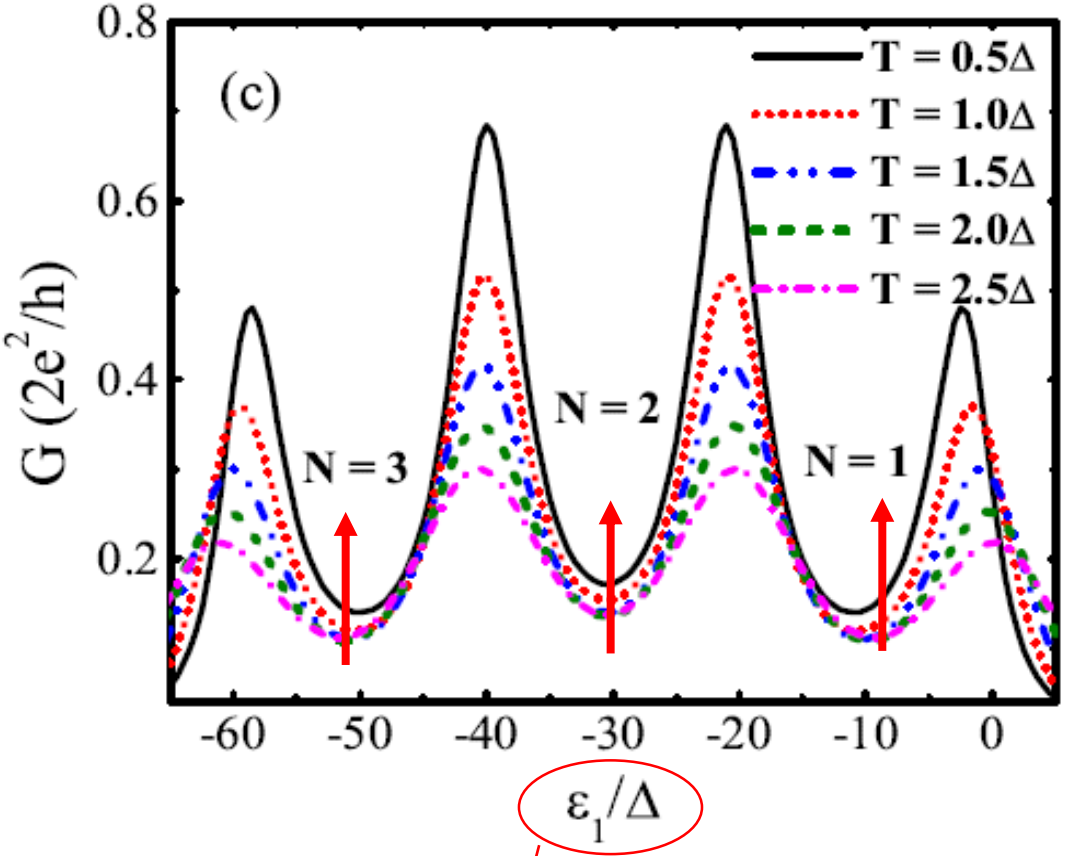
$$|00>, |u0>, |d0>, |20>,$$
$$|0u>, |uu>, |du>, |2u>,$$
$$|0d>, |ud>, |dd>, |2d>,$$
$$|02>, |u2>, |d2>, |22>$$



Example: steady state calculations

convergence test! and then

- Calculation of conductance of two-level QDs

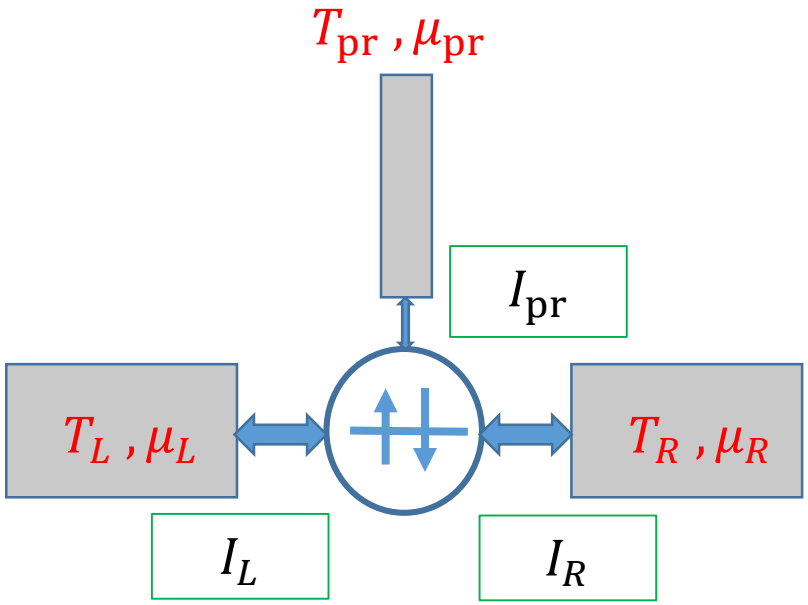


by varying e1up, e1down, e2up and e2down

Single-level QD coupled with 3 leads

Quantum Dot (QD)
Left/Right leads
an additional lead -- the probe

electric current: $I_\alpha, \alpha = L, R, \mathrm{pr}$



- single impurity Anderson model

$$H_{\mathrm{dot}} = \epsilon_\uparrow n_\uparrow + \epsilon_\downarrow n_\downarrow + U n_\uparrow n_\downarrow \qquad (n_s = a_s^+ a_s)$$

Sample input file

```
     2
     3
    10
     1
     2
     3
 0.80000000E+01   0.80000000E+01   0.80000000E+01
 0.10000000E+00   0.10000000E+00   0.10000000E-02
  0.130000E-001    0.130000E-001   0.008d0
-0.24121728E-01  -0.24121728E-01   0.24121728E-01   0.24121728E-01   0.00000000E+00   0.00000000E+00
  0.100000E+004
  0.200000E-001

 $para1  eup=   -0.086000  edown=   -0.086000  uu=    5.000000  fixdot=.true. $end

 $field  fieldtype= 0  $end
 0.10000000E-19   0.10000000E-19   0.10000000E-19   0.10000000E-19   0.10000000E-19   0.10000000E-19

 $jobinfo  lsparse=T  $end
```

# of leads = 3

band width W_1, W_2, W_3

dot-lead coupling $\Delta_1, \Delta_2, \Delta_3$

temperature T_1, T_2, T_3

energyshift/voltage $V_{1\uparrow}, V_{1\downarrow}, V_{2\uparrow}, V_{2\downarrow}, V_{3\uparrow}, V_{3\downarrow}$

output file

electric current:

```
   j(ialf =          1  )=   -1502.95810196406       pA
   j(ialf =          2  )=    1498.65567336029       pA
   j(ialf =          3  )=    4.30194315971913       pA

 j_up  (ialf =           1  )=   -751.479051302878       pA
 j_down(ialf =           1  )=   -751.479050661178       pA
 j_up  (ialf =           2  )=    749.327836936592       pA
 j_down(ialf =           2  )=    749.327836423693       pA
 j_up  (ialf =           3  )=    2.15097130063586       pA
 j_down(ialf =           3  )=    2.15097185908327       pA
```

$$I_1 + I_2 + I_3 = 0$$

$$I_{i\uparrow} = I_{i\downarrow} \quad , i = 1, 2, 3$$

spin-degenerate, eup = edown

```
$para1  eup=   -0.086000  edown=   -0.086000  uu=    5.000000  fixdot=.true. $end
```

Spectral function

➢ Dot spectral function $A(\omega)$

definition: $A_i(\omega) \equiv \frac{1}{2\pi}\int dt\, e^{i\omega t}\,\langle\{\hat{a}_i(t), \hat{a}_i^{\dagger}(0)\}\rangle$

single-level QD, $i = 1$

two-level QD, $i = 1, 2$

n-level QD, $i = 1, 2, \cdots, n$

for spin-degenerate model,

$$A_{i\uparrow}(\omega) = A_{i\downarrow}(\omega)$$

if not, $A_{i\uparrow}(\omega) \neq A_{i\downarrow}(\omega)$

nonequilibrium, electric current, heat current, energy current --- the spectra in frequency domain

Single-electron Green functions

$$G^r_{ij}(t) \equiv -i\theta(t)\,\langle\{\hat{a}_i(t), a^\dagger_j(0)\}\rangle = -i\theta(t)\left[C_{\hat{a}_i\hat{a}^\dagger_j}(t) + C_{\hat{a}^\dagger_j\hat{a}_i}(-t)\right]$$

$$G^<_{ij}(t) \equiv \langle\hat{a}_j(0)a^\dagger_i(t)\rangle = iC_{\hat{a}^\dagger_j\hat{a}_i}(-t)$$

Stationary electric and heat currents

Meir and Wingreen, *PRL* **68**, 2512 (1992)

$$I_\alpha = \frac{ie}{h}\int d\epsilon\, 2\Delta_\alpha(\epsilon)\Big\{G^<(\epsilon) + 2\,i f_\alpha(\epsilon)\,\mathrm{Im}\,[G^r(\epsilon)]\Big\}$$

$$J^{\mathrm{H}}_\alpha = \frac{i}{h}\int d\epsilon\,(\epsilon-\mu_\alpha)\,2\Delta_\alpha(\epsilon)\Big\{G^<(\epsilon) + 2\,i f_\alpha(\epsilon)\,\mathrm{Im}\,[G^r(\epsilon)]\Big\}$$

and energy current:

$$J^{\mathrm{E}}_\alpha = \frac{i}{h}\int d\epsilon\,\epsilon\,\Gamma_\alpha(\epsilon)\Big\{G^<(\epsilon) + 2\,i\,f_\alpha(\epsilon)\,\mathrm{Im}[G^r(\epsilon)]\Big\},$$

for lead-α

$J^E_\alpha = J^H_\alpha + \mu_\alpha I_\alpha/e$, where $e = -q_e = -1.602\times10^{-19}\mathrm{C}$

Sample input file for single-level QD


```
     3   3 for spectral function
     3
    11
     1
     2
     2
0.30000000E+01    0.30000000E+01
0.10000000E+00    0.10000000E+00
0.20000000E-01    0.20000000E-01
0.00000000E+00    0.00000000E+00    0.00000000E+00    0.00000000E+00
0.10000000E+04
0.20000000E-01

$para1  eup=   -0.450000  edown=   -0.450000  uu=    1.000000  fixdot=T $end

$field  fieldtype= 0  $end
0.10000000E-19    0.10000000E-19    0.10000000E-19    0.10000000E-19

$dos ldos=T  iorbs_dos=1  ispin_dos=1
   lfreq_dos=T  freq_dos=-0.220
     crit_dos=1.000E-005 $end

$combineleads lequileads=T $end
$jobinfo  lsparse=T  $end
```

iorbs_dos = 1 : 1 for level-1
ispin_dos = 1 : 1 for spin-up, 2 for spin-down
lfreq_dos=T : in frequency ω domain
freq_dos=-0.220 : value of $A(\omega = -0.220)$
crit_dos = 1e-5 : convergence criterion is 1e-5

combineleads lequileads=T: combine the leads when leads are identical,

identical leads means: same bandwidth, temperature, and engyshift=0

see ./readme/HISTORY.log

output file

equilibrium, $V = 0$

```
CORRFUNC_ AW    -0.220000E+000   0.405401E+000   0.458724E+000   -0.533234E-001
```

$\omega = -0.22$

$A(\omega)$

```
CORRFUNC_ IW    -0.220000E+000   -0.258237E+001
CORRFUNC_ JHW   -0.220000E+000   -0.568122E+000
CORRFUNC  JEW   -0.220000E+000   -0.568122E+000
```

electric current
heat current
energy current

for lead-1

nonequilibrium, e.g. $V = V_L - V_R = 0.2$

```
0.1   0.1   -0.1   -0.1
```

voltage

```
$combineleads lequileads=F $end
```

output file

```
CORRFUNC_ AW      -0.220000E+000    0.436277E+000    0.483744E+000   -0.474668E-001

CORRFUNC_ IW      -0.220000E+000   -0.114241E+001   -0.117978E+001
CORRFUNC_ JHW     -0.220000E+000   -0.365571E+000   -0.141573E+000
CORRFUNC  JEW     -0.220000E+000   -0.251330E+000   -0.259551E+000
```

for lead-1

for lead-2

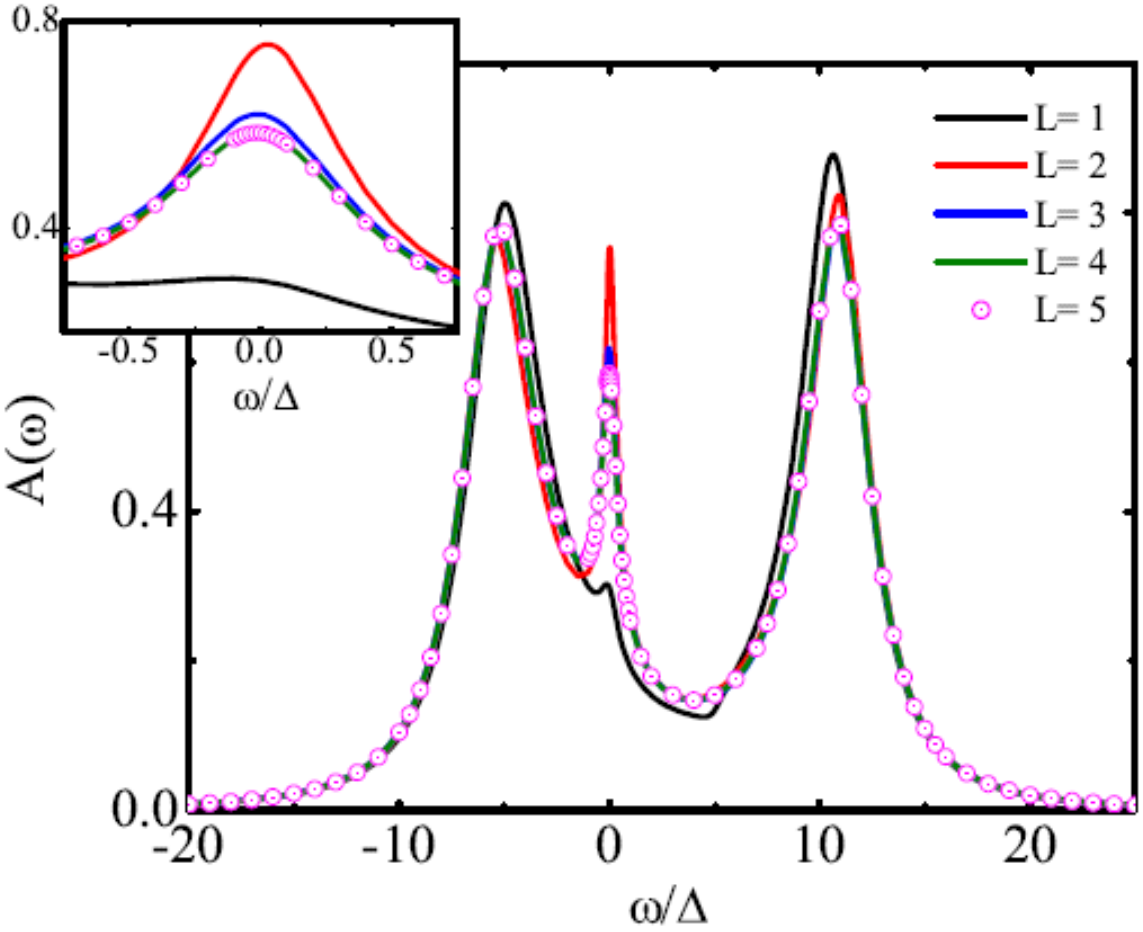
usually, if $A(\omega)$ converges at L

then $I(\omega), JH(\omega), \text{and } JE(\omega)$ should converge at $L + 1$

BE CAREFULL!

convergence test

spectral function $A(\omega)$ vs. truncation level L



Sample input file for two-level QD


```
   3
   5
  10
   2
   2
   2
0.800000E+001    0.800000E+001
0.100000E+000    0.100000E+000    0.100000E+000    0.100000E+000
0.500000E-001    0.500000E-001
0.000000E+000    0.000000E+000    0.000000E+000    0.000000E+000
0.100000E+004
0.200000E-001
 $hamil_sys  lgenhs=.true.$end
 hsys
 edot  1  1     -6.5500
 edot  2  1     -6.5500
 edot  1  2     -6.4500
 edot  2  2     -6.4500
 udot  0  1      2.0000
 udot  0  2      2.0000
 ucoup  0  2  1      2.0000
 $jobinfo lsparse=T  $end

 $field  fieldtype= 0  $end
  0.100000E-019    0.100000E-019    0.100000E-019    0.100000E-019


 $dos ldos=T  iorbs_dos=1  ispin_dos=1
    lfreq_dos=T  freq_dos=-0.120
      crit_dos=1.000E-005 $end

 $combineleads lequileads=T $end
```

you should calculate $A_1(\omega), A_2(\omega)$, for level-1 and level-2, respectively

iorbs_dos=1 ispin_dos=1 for $A_{1\uparrow}(\omega)$

iorbs_dos=1 ispin_dos=2 for $A_{1\downarrow}(\omega)$

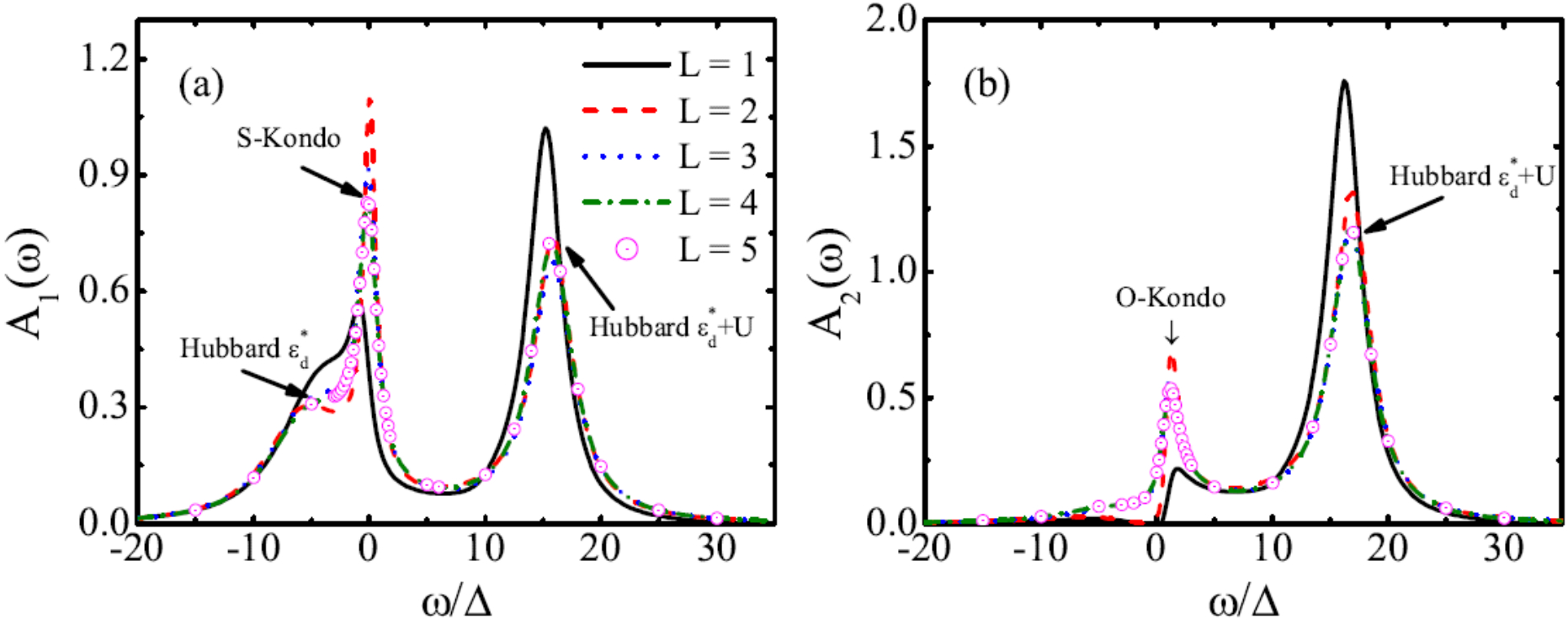
iorbs_dos=2 ispin_dos=1 for $A_{2\uparrow}(\omega)$

iorbs_dos=2 ispin_dos=2 for $A_{1\downarrow}(\omega)$

Thermopower of two-level QD

- Convergence vs truncation level L

spectral function $A_i(\omega)$ of level-1 and level-2



Thank You!