Impurity problems away from equilibrium: A hierarchical quantum master equation approach

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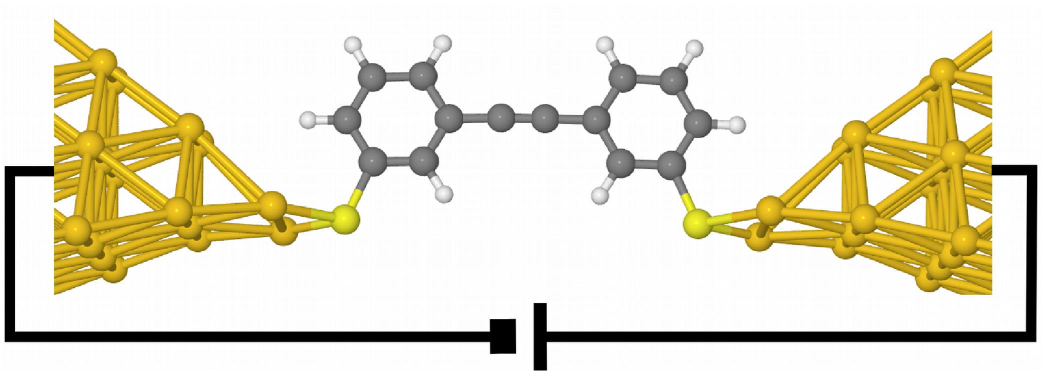
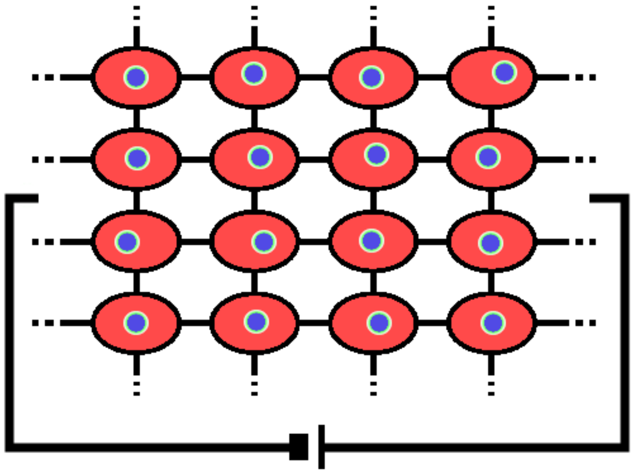
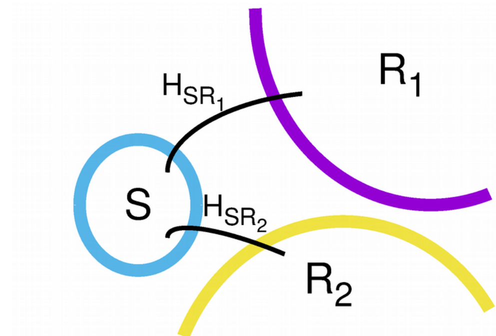
Georg-August-Universität Göttingen





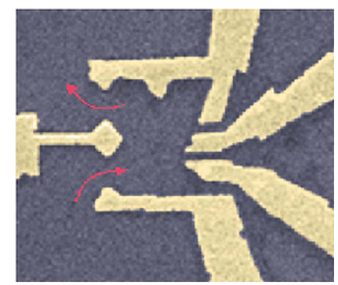
Outline

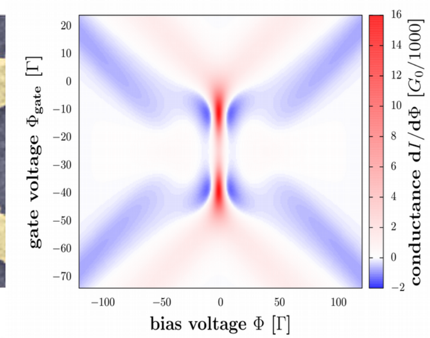
- Model Hamiltonian



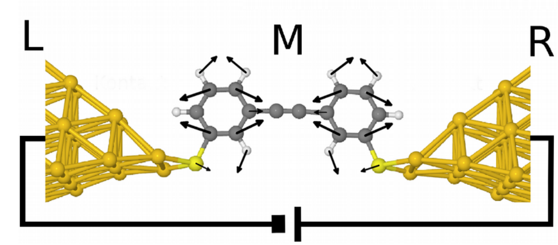
- Hierarchical quantum master equation approach

- Sharp peaks in the conductance-voltage characteristics for T»T_{Kondo}

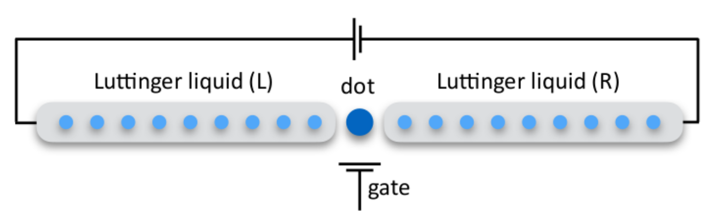




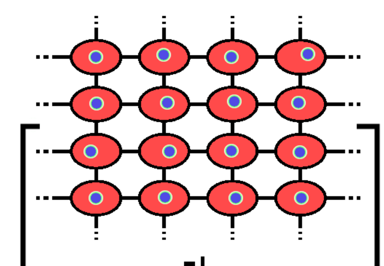
- Crossover in inelastic electron tunneling spectra (IETS)



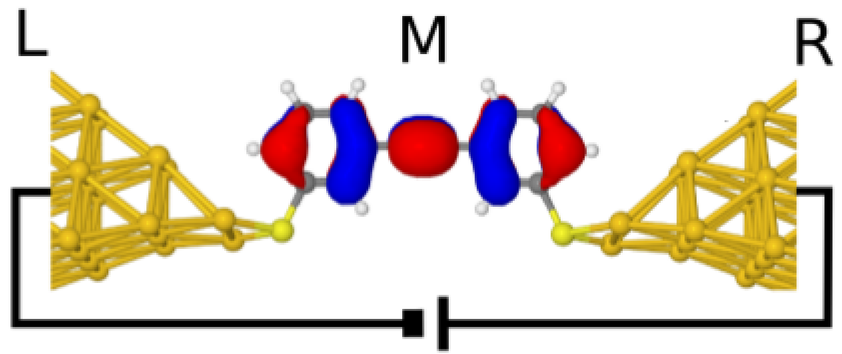
- Negative diff. resistance with Luttinger liquid leads



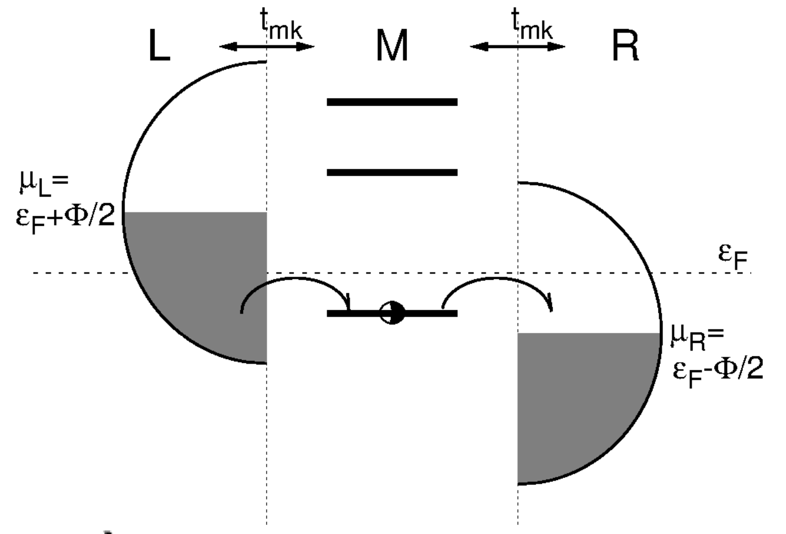
- Transport characteristics of a correlated material



Model Hamiltonian



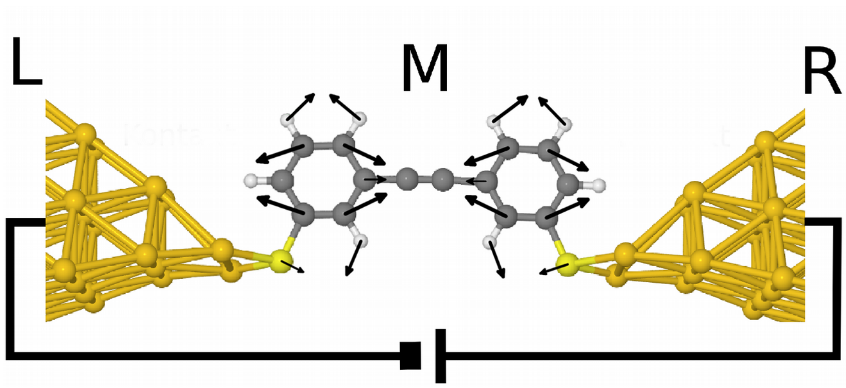
$$H_{\text{imp}} = \sum_m \epsilon_m d_m^\dagger d_m + \sum_{m>n} U_{mn} d_m^\dagger d_m d_n^\dagger d_n$$



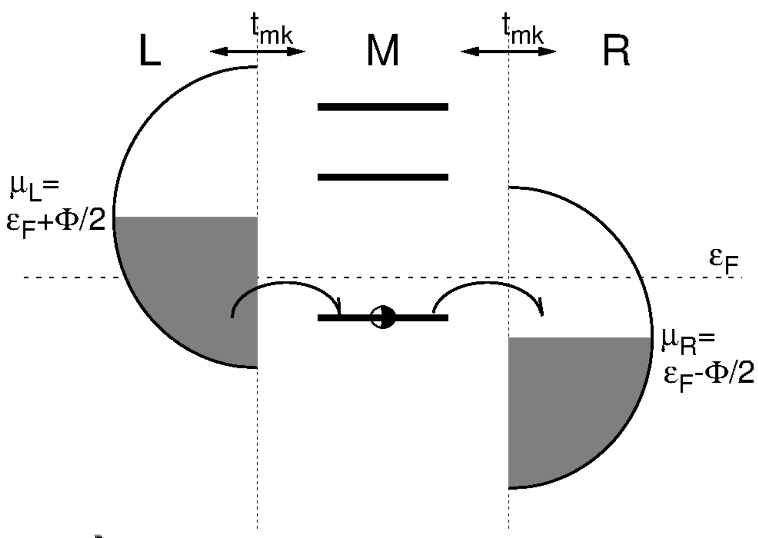
$$H_{\text{env}} = \sum_k \epsilon_k c_k^\dagger c_k,$$

$$H_{\text{tun}} = \sum_{k;m} (V_{kn} c_k^\dagger d_m + \text{h.c.}).$$

Model Hamiltonian



$$H_{\text{imp}} = \sum_m \epsilon_m d_m^\dagger d_m + \sum_{m>n} U_{mn} d_m^\dagger d_m d_n^\dagger d_n$$
$$+ \sum_{m\alpha} \lambda_{m\alpha} d_m^\dagger d_m (a_\alpha + a_\alpha^\dagger)$$
$$+ \sum_\alpha \Omega_\alpha a_\alpha^\dagger a_\alpha$$



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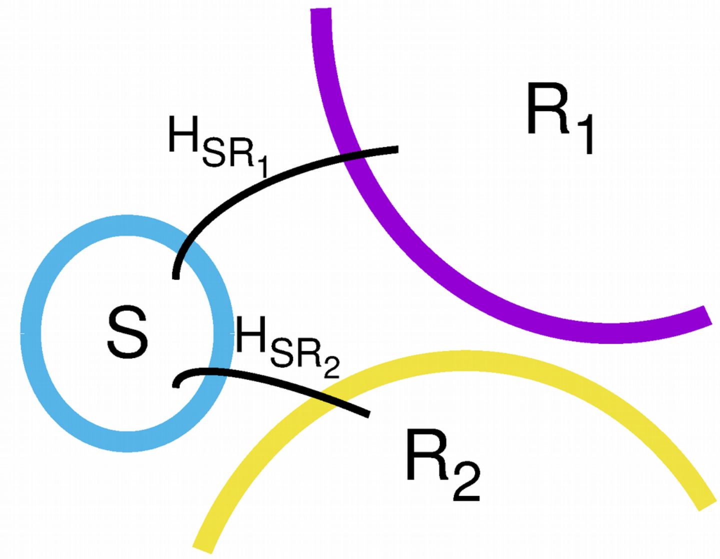
Hierarchical master equations

EOM for impurity density matrix ρ
(H_{env}-interaction picture)

$$\partial_t \rho(t) = -i\left[H_{\mathrm{imp}}, \rho(t)\right] - i\tilde{\rho}(t)$$

with $\tilde{\rho}(t) = \mathrm{Tr}_{\mathrm{env}}\left\{[H_{\mathrm{tun}}(t), \varrho(t)]\right\}$

and $\varrho(0) = \rho_{\mathrm{env}}\rho$.



$$\begin{aligned}\tilde{\rho}(t) = \textstyle\sum_{K\in\{\mathrm{env}\},mn,s\in\{+,-\}} \int_0^t \mathrm{d}\tau\, C^s_{K,mn}(t-\tau)\times \\ \Big(\Big[d^{\bar{s}}_m, \mathrm{Tr}_{\mathrm{env}}\left\{U(t,\tau)d^s_n U(\tau,0)\varrho(0)U^\dagger(t,0)\right\}\Big] \\ -\Big[d^{\bar{s}}_m, \mathrm{Tr}_{\mathrm{env}}\left\{U(t,0)\varrho(0)U^\dagger(\tau,0)d^s_n U^\dagger(t,\tau)\right\}\Big]\Big),\end{aligned}$$

with $C^s_{K,mn}(t-\tau) = \sum_{k\in K} V^{\bar{s}}_{mk} V^s_{nk} \mathrm{Tr}_K \left\{\rho_K c^s_k(t) c^{\bar{s}}_k(\tau)\right\}, s = \pm.$

Tanimura and Kubo ’89/’90; Jin *et al.*, JCP **128**, 234703 (2008).

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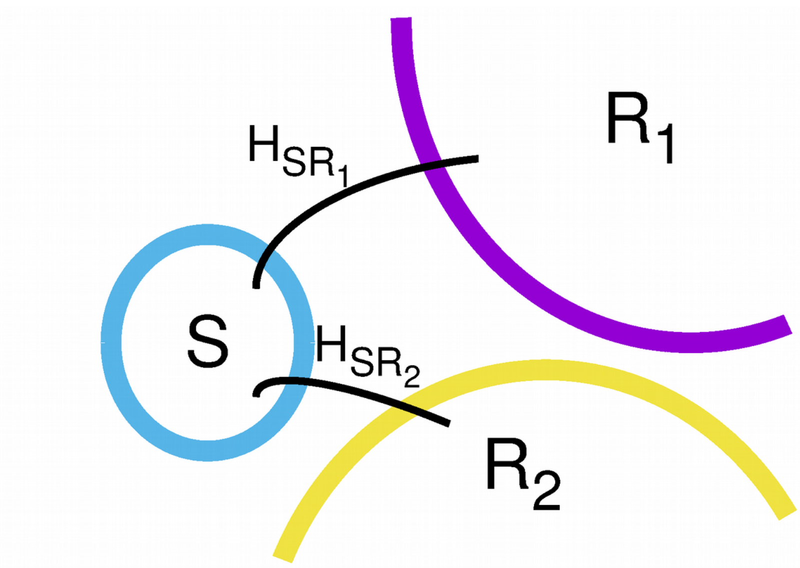

$$\begin{aligned}\tilde{\rho}(t) = \textstyle\sum_{K,mn,s,p} \int_0^t \mathrm{d}\tau\, \eta^{s}_{R_r,mn,p} \mathrm{e}^{-\omega^{s}_{R_r,p}(t-\tau)} \times \\ \Big(\Big[d^{\bar{s}}_m, \mathrm{Tr}_{\mathrm{env}}\left\{U(t,\tau) d^{s}_n U(\tau,0)\varrho(0)U^{\dagger}(t,0)\right\}\Big] \\ -\Big[d^{\bar{s}}_m, \mathrm{Tr}_{\mathrm{env}}\left\{U(t,0)\varrho(0)U^{\dagger}(\tau,0) d^{s}_n U^{\dagger}(t,\tau)\right\}\Big]\Big),\end{aligned}$$

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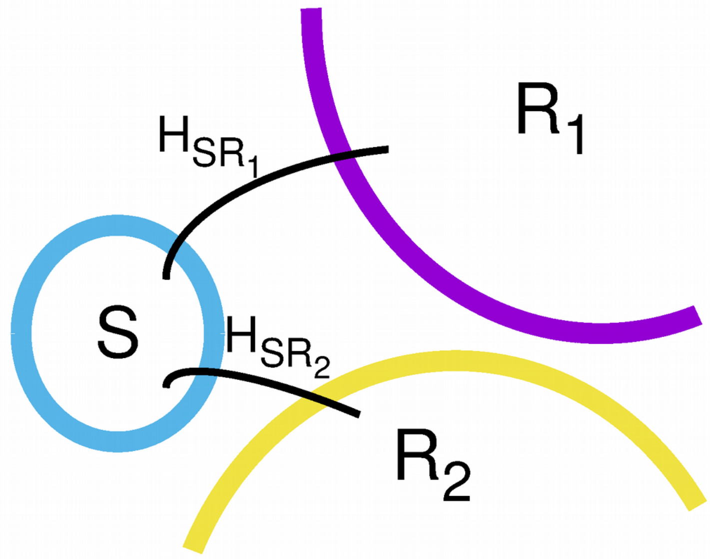

Closed hierarchy of time-local EOMs:

$$\partial_t \rho^{(\alpha)}_{j_1..j_\alpha}(t) = -i\left[H_{\text{imp}}, \rho^{(\alpha)}_{j_1..j_\alpha}(t)\right] - \sum_{\beta\in\{1..\alpha\}} \omega_{j_\beta}\rho^{(\alpha)}_{j_1..j_\alpha}(t)$$

$$+\sum_\beta (-1)^{\alpha-\beta}\eta_{j_\beta} d^{s_\beta}_{\sigma_\beta}\rho^{(\alpha-1)}_{j_1..j_\alpha/j_\beta}(t) + (-)^\beta \eta^*_{\bar{j_\beta}}\rho^{(\alpha-1)}_{j_1..j_\alpha/j_\beta}(t) d^{s_\beta}_{\sigma_\beta}$$

$$-\sum_{j_{\alpha+1},\sigma_{\alpha+1}} d^{\bar{s}_{\alpha+1}}_{\sigma_{\alpha+1}}\rho^{(\alpha+1)}_{j_1..j_\alpha j_{\alpha+1}}(t) - (-1)^\alpha \rho^{(\alpha+1)}_{j_1..j_\alpha j_{\alpha+1}}(t) d^{\bar{s}_{\alpha+1}}_{\sigma_{\alpha+1}}.$$

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Hierarchical master equations

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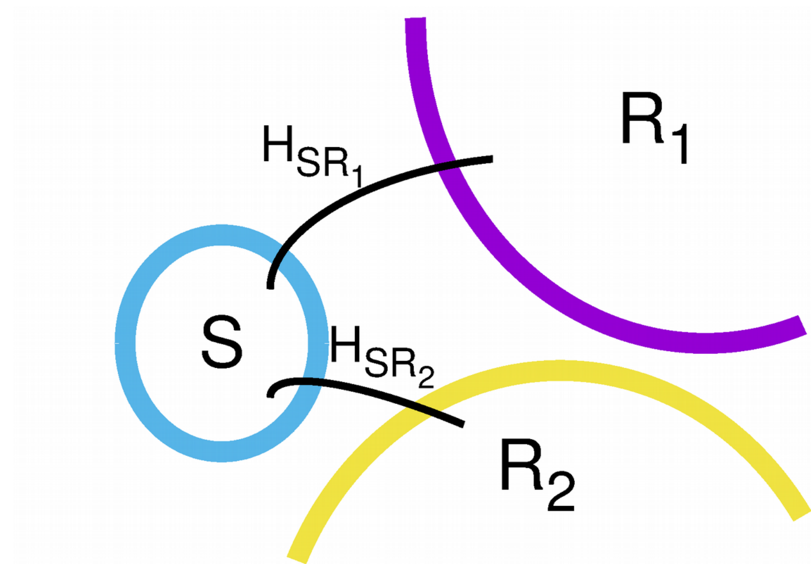
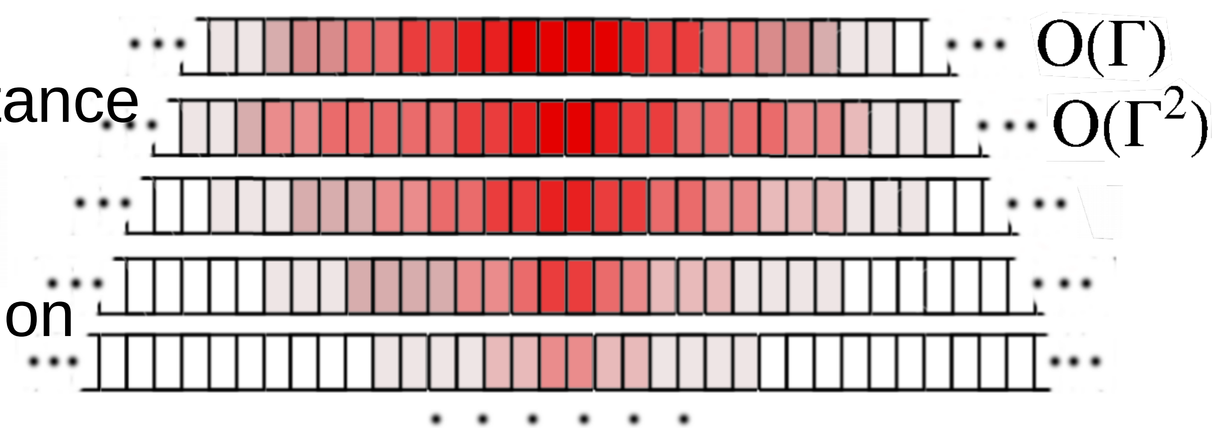


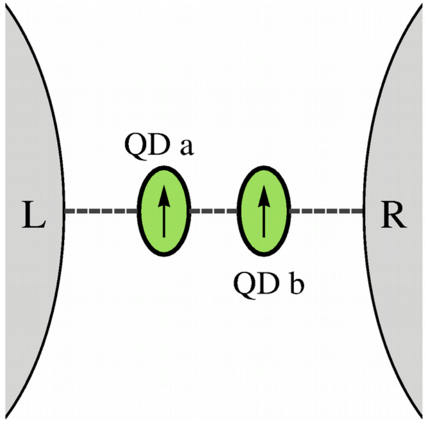
Estimate importance
of the $\rho^{(\alpha)}_{j_1..j_\alpha}(t)$
prior to calculation

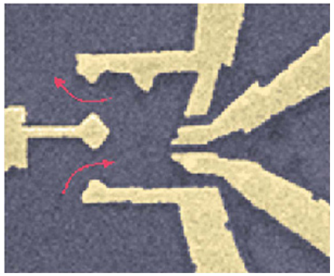


$\rightarrow$ optimized hybridization expansion w.r.t. temperature scale.

$\rightarrow$ exact when converged, Härtle *et al.*, PRB **88**, 235426 (2013).
cf. QMC, Härtle *et al.*, PRB **92**, 245426 (2015).

Sharp conductance peaks



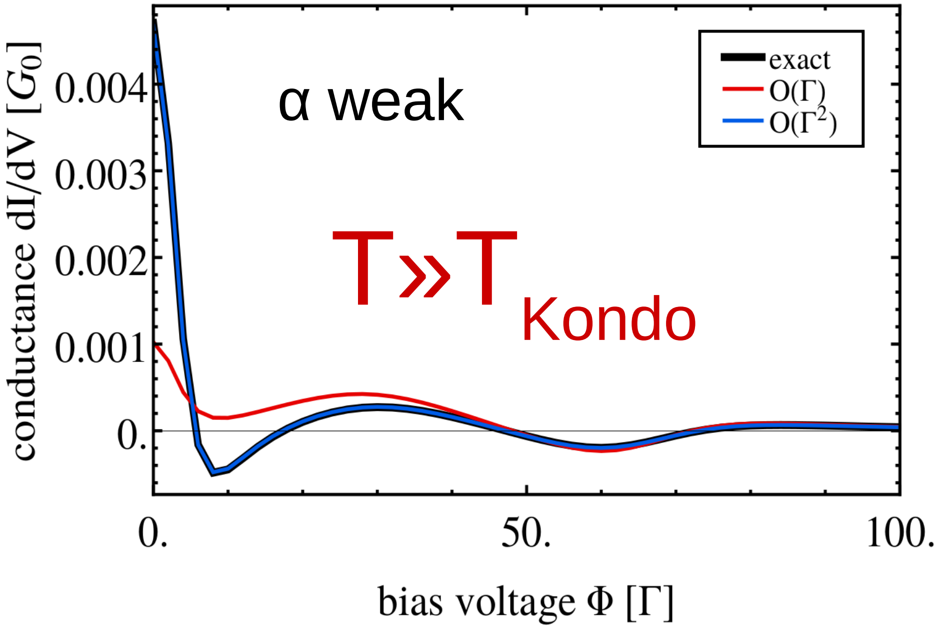


$$\Gamma_L = \Gamma_R$$

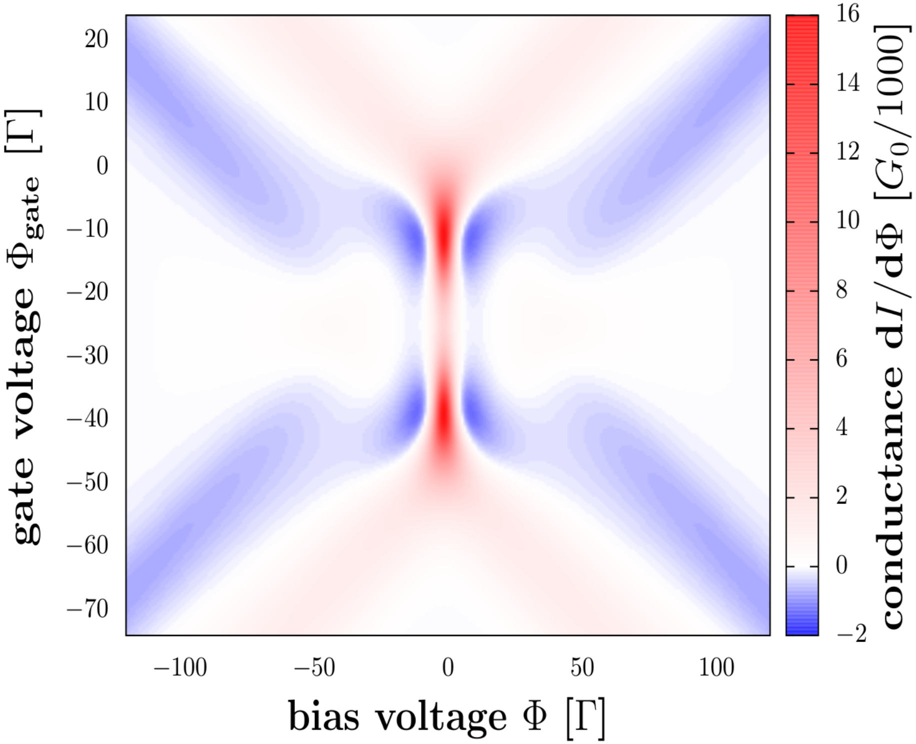
$$H_{DQD} = \sum_{m\in a,b} \epsilon_m d_m^\dagger d_m$$
$$\alpha(d_a^\dagger d_b + h.c.) + U d_a^\dagger d_a d_b^\dagger d_b$$

$$H_{L+R} = \sum_{k\in L,R} \epsilon_k c_k^\dagger c_k$$

$$H_{tun} = \sum_{m,k} V_{mk} c_k^\dagger d_m + h.c.$$



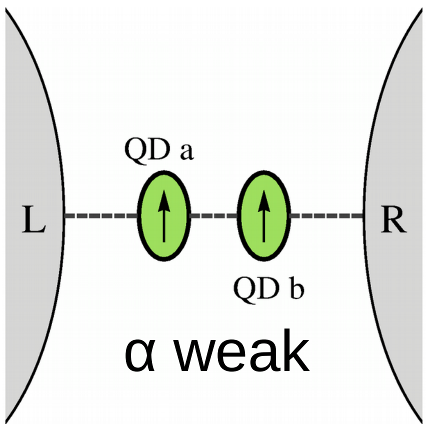
Renormalization due to exchange interactions

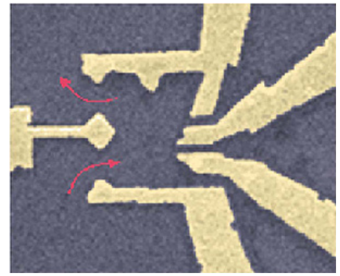


$$\Delta_{a/b} = \frac{\Gamma}{2\pi}\mathrm{Re}\left[\Psi\left(\frac{1}{2} + \frac{i(\epsilon_{a/b}-\mu_{L/R})}{2\pi T}\right)\right] - \frac{\Gamma}{2\pi}\mathrm{Re}\left[\Psi\left(\frac{1}{2} + \frac{i(\epsilon_{a/b}+U-\mu_{L/R})}{2\pi T}\right)\right]$$

Martinek, König, PRL90, 166602 (2003)
RH, Millis, PRB 90, 245426 (2014)
Wenderoth, Bätge, RH, PRB 94, 121303R (2016)

Sharp conductance peaks





$$\Gamma_L = \Gamma_R$$

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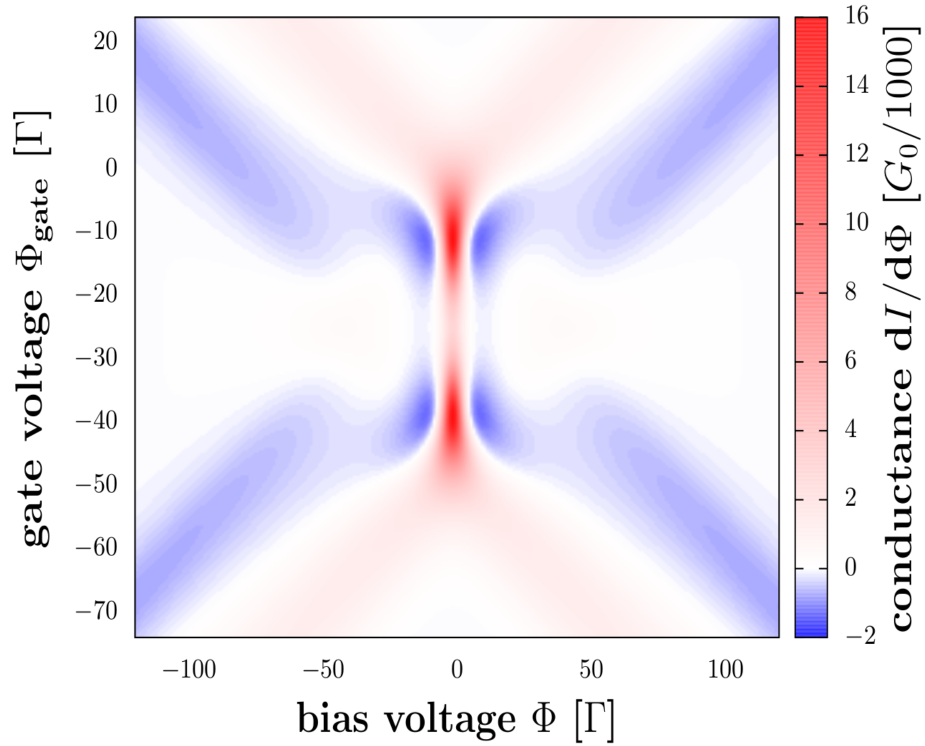

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$$\alpha(d_a^\dagger d_b + h.c.) + U d_a^\dagger d_a d_b^\dagger d_b$$

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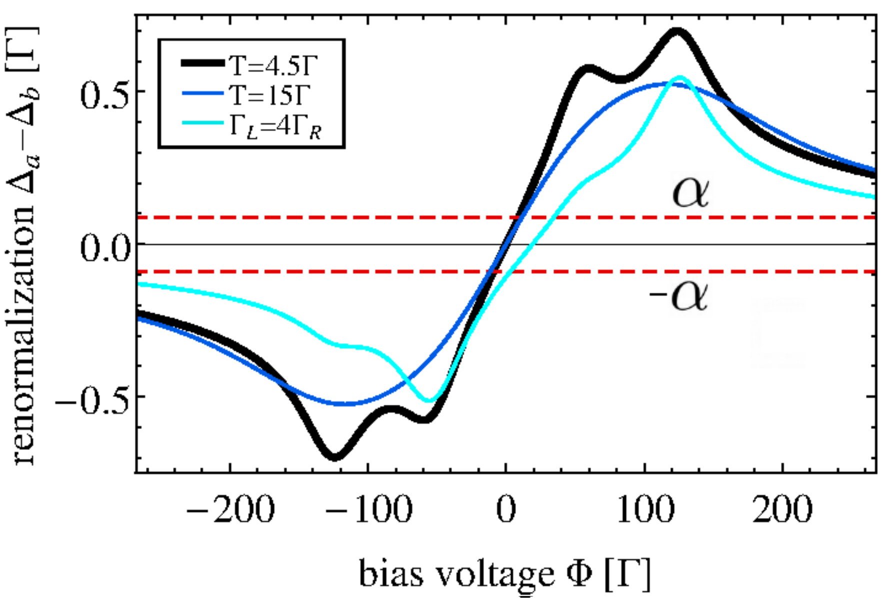

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RH, Millis, PRB 90, 245426 (2014)
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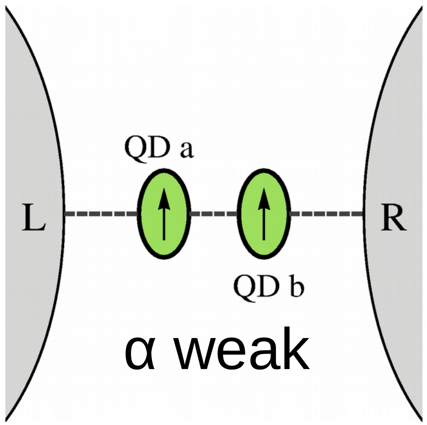
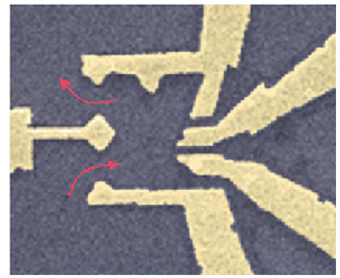
Sharp conductance peaks

Long times scales $t \sim 10^2$–$10^3\Gamma$





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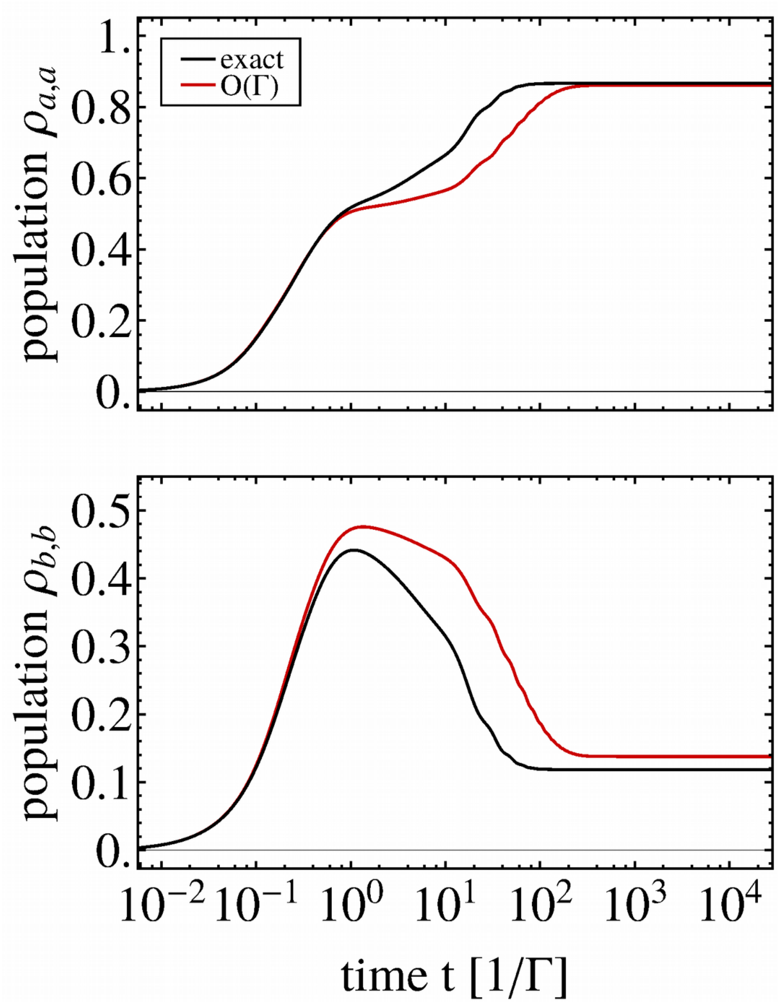

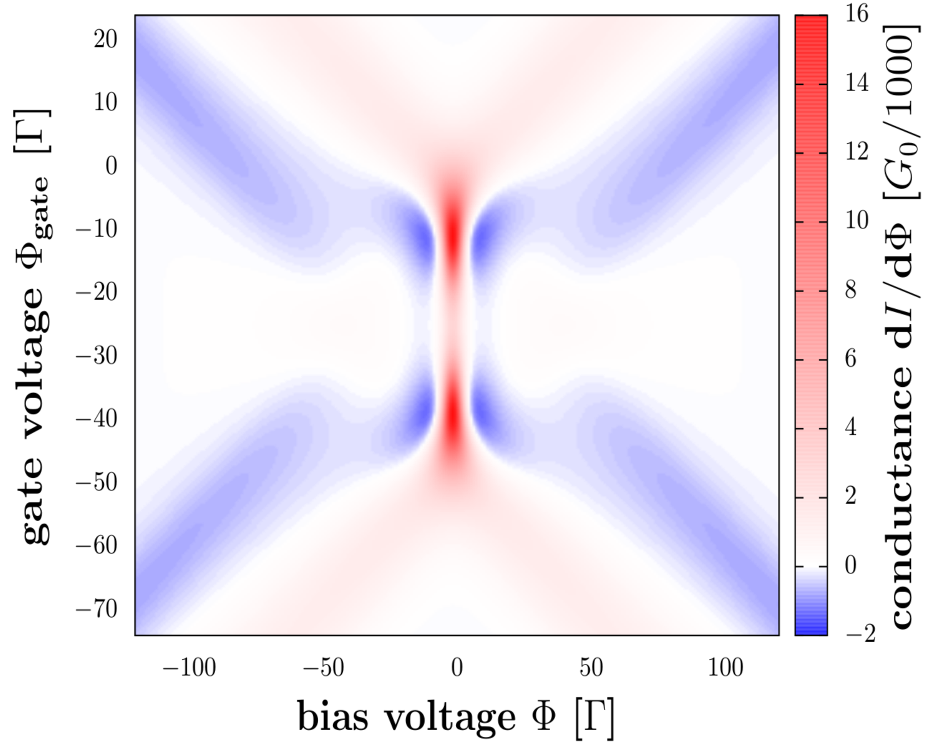

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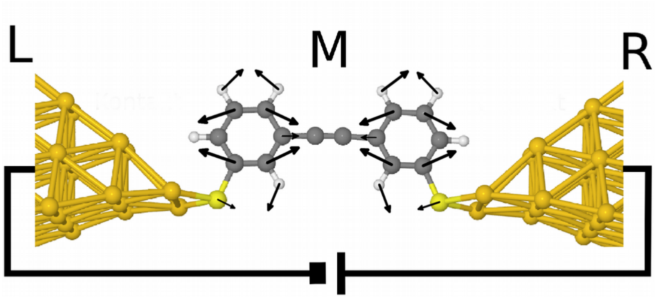
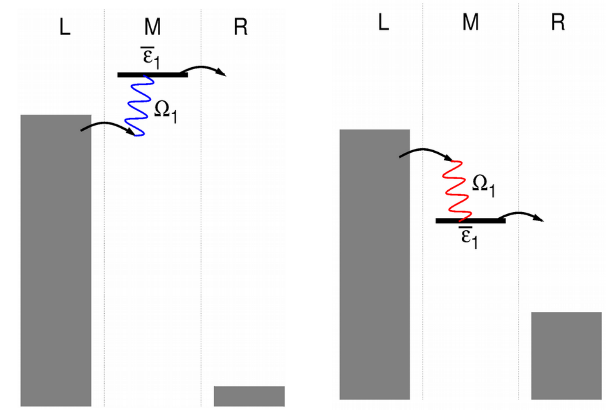


Vibrational cross-over regime

Steps at
$\Phi=2(\varepsilon_0+n\Omega)$



$$H_{QD} = (\epsilon_0 + \lambda(a + a^\dagger))d^\dagger d + \Omega a^\dagger a$$

$$H_{L+R} = \sum_{k\in L,R} \epsilon_k c_k^\dagger c_k$$

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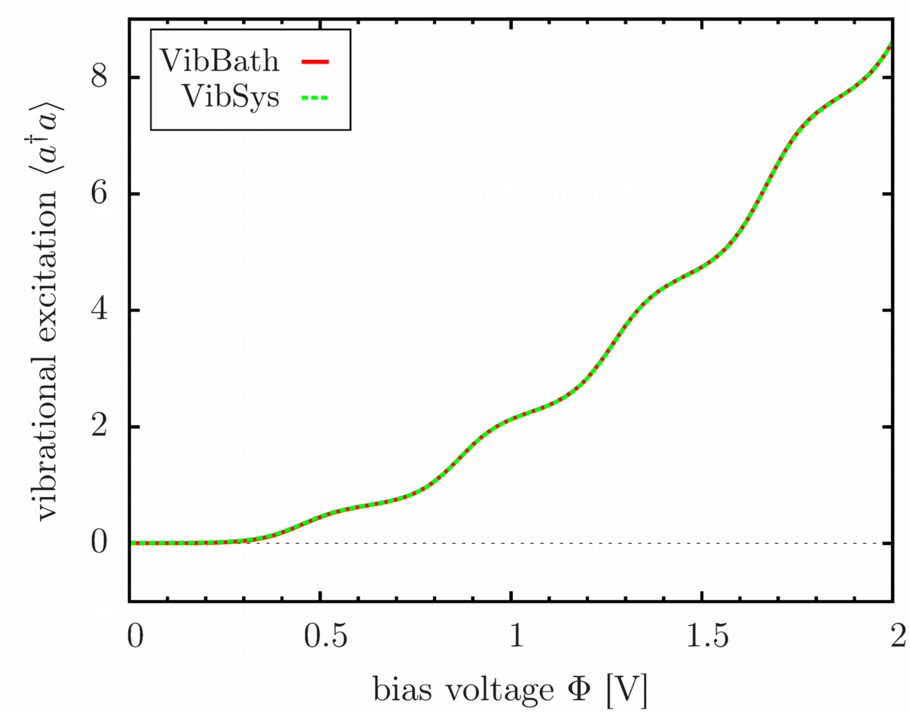
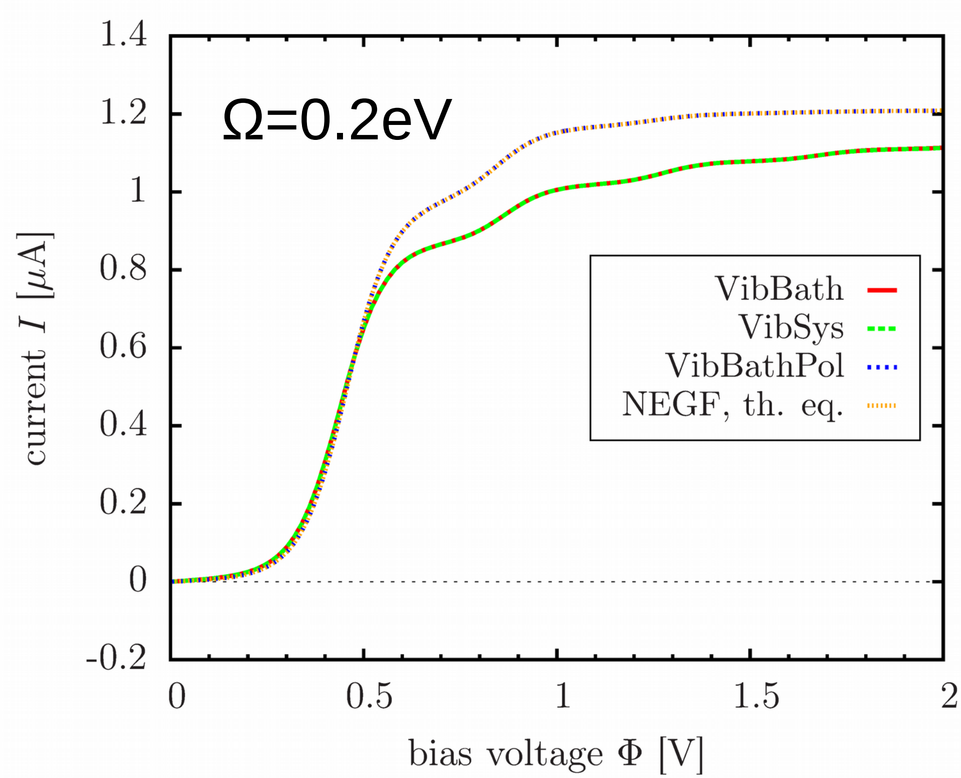
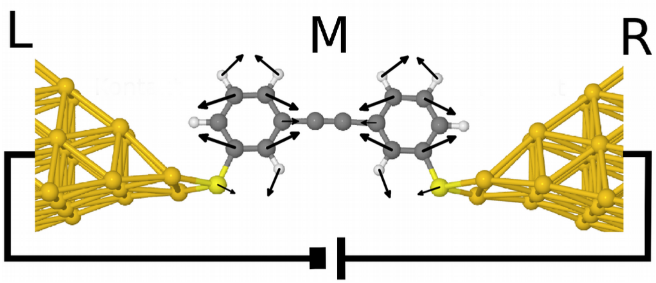


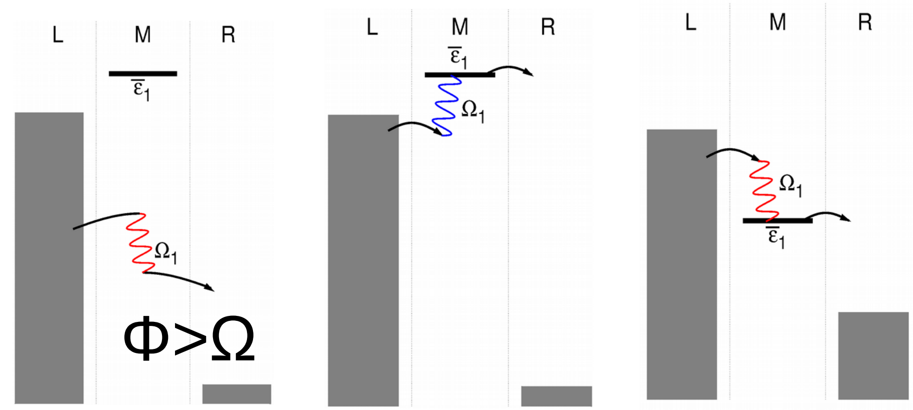


Schinabeck, Erpenbeck, RH, Thoss, arXiv:1609.05149 (2016)



Vibrational cross-over regime

kinks at
$\Phi > n\Omega$



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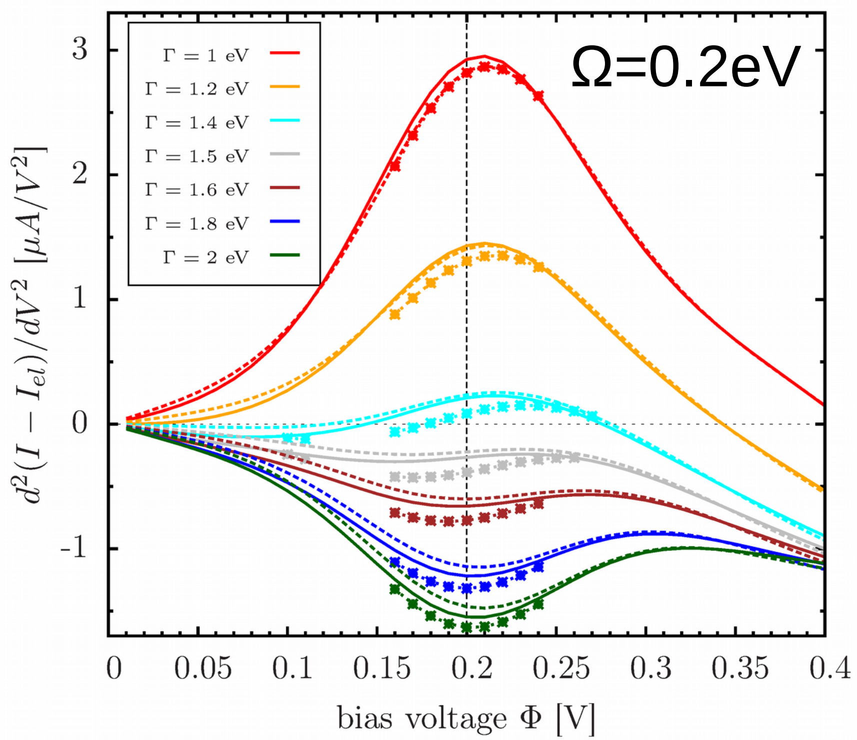

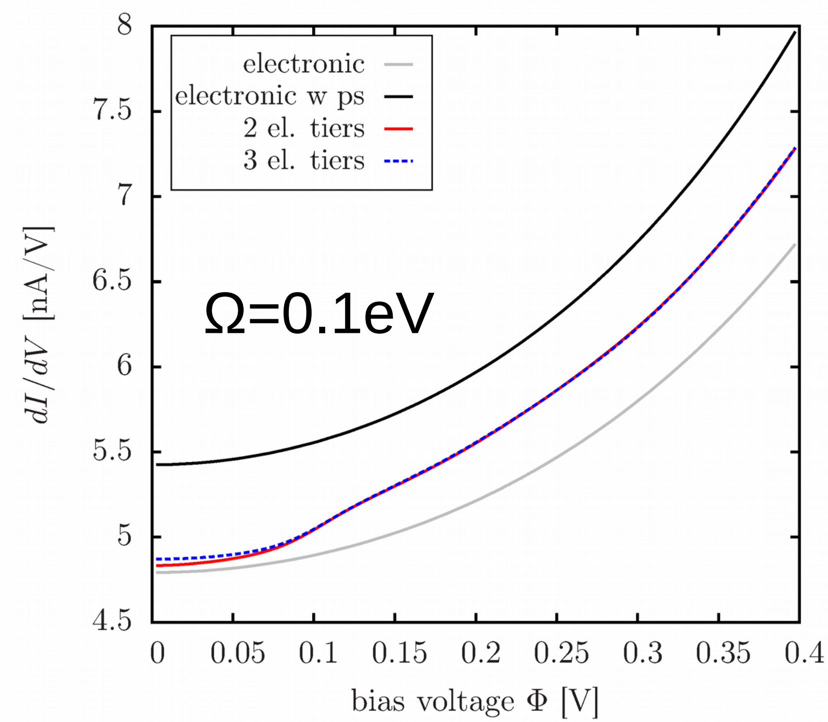

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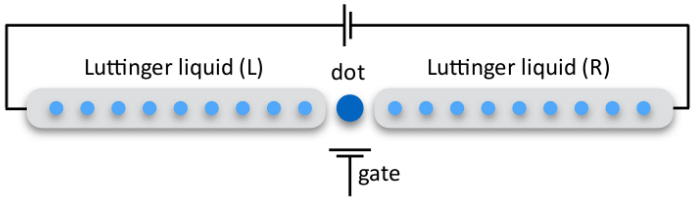
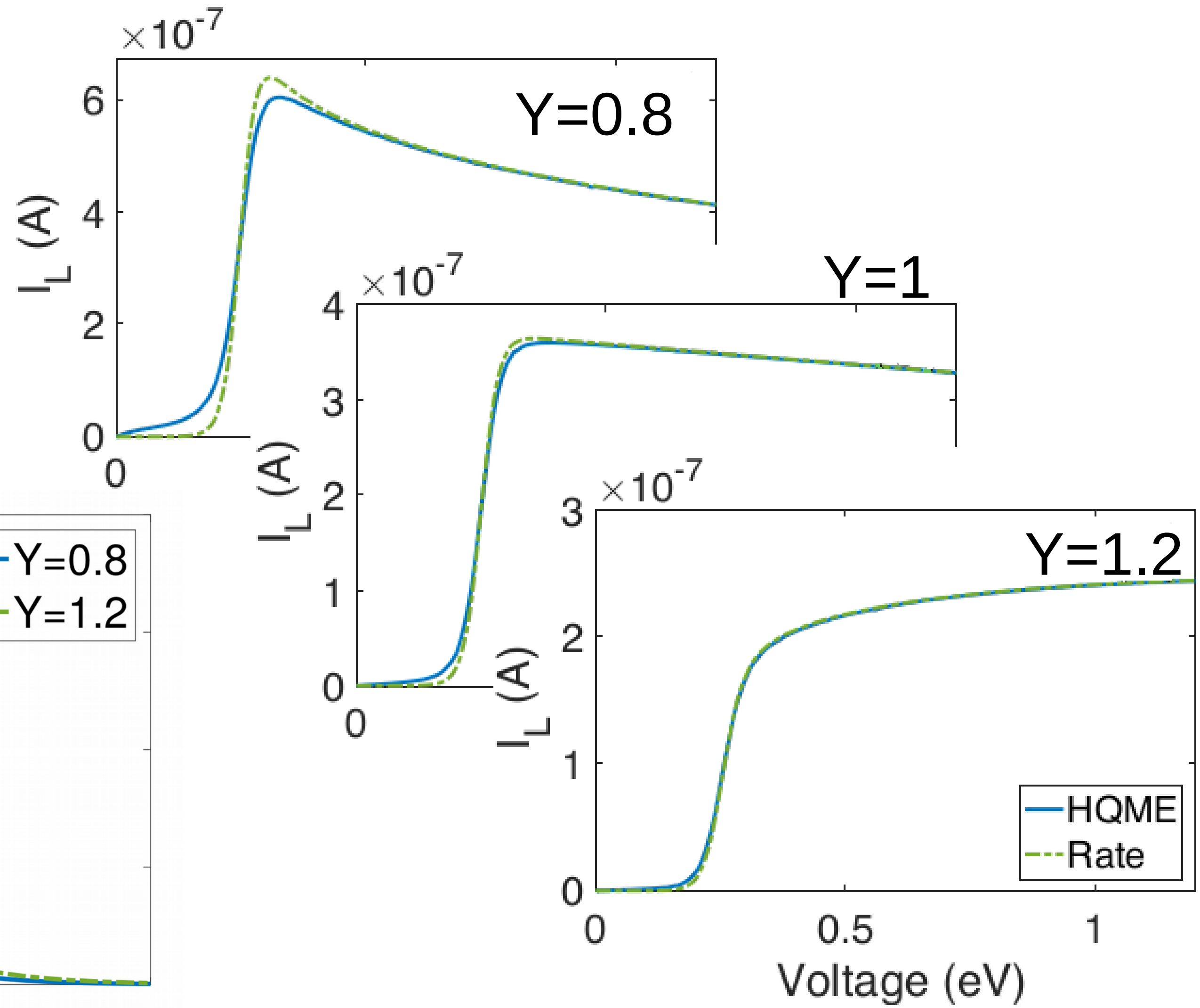


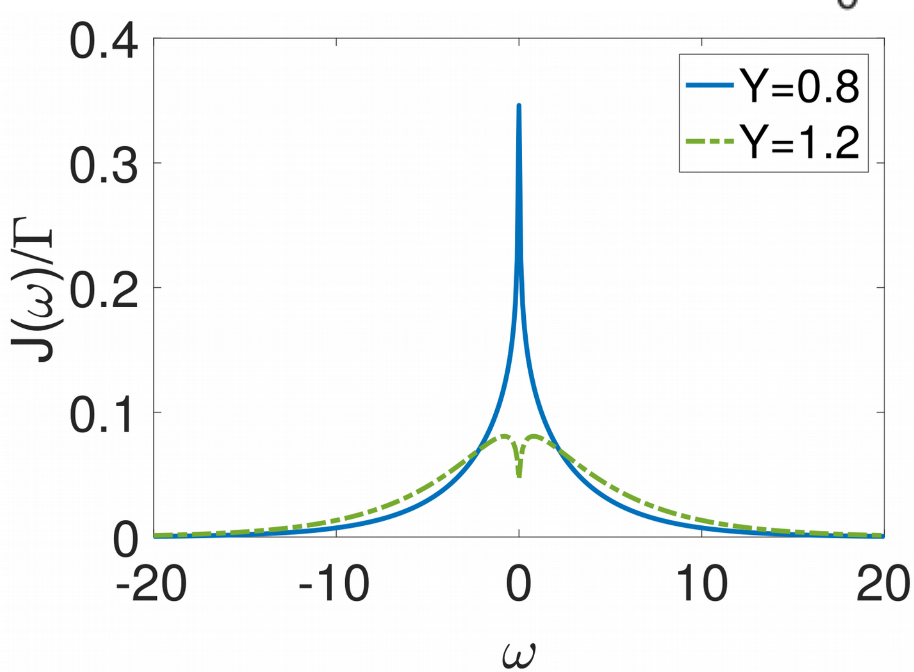
Luttinger liquid leads

$$H^{\alpha}_{\text{lead}} = \sum_{\nu=c,s} \frac{1}{2\pi} \int dx \left[u^{\alpha}_{\nu} K^{\alpha}_{\nu} \left(\nabla\theta^{\alpha}_{\nu}\right)^2 + \frac{u^{\alpha}_{\nu}}{K^{\alpha}_{\nu}} \left(\nabla\phi^{\alpha}_{\nu}\right)^2 \right]$$

Interactions renormalize tunneling efficiency J(ω)
→ negative differential resistance (NDR)

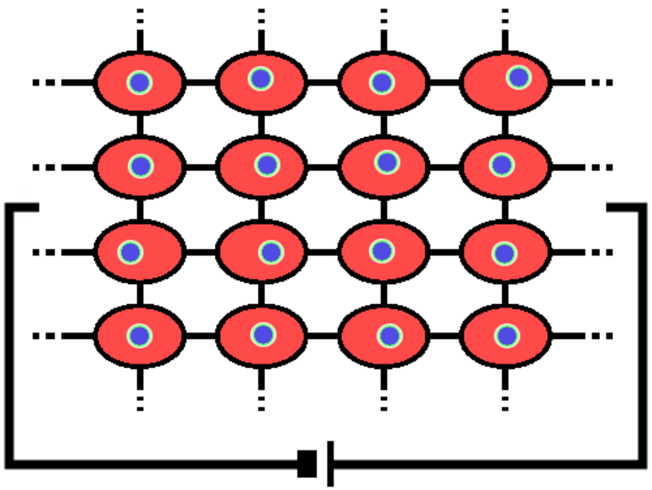
Two-particle correlations are negligible here





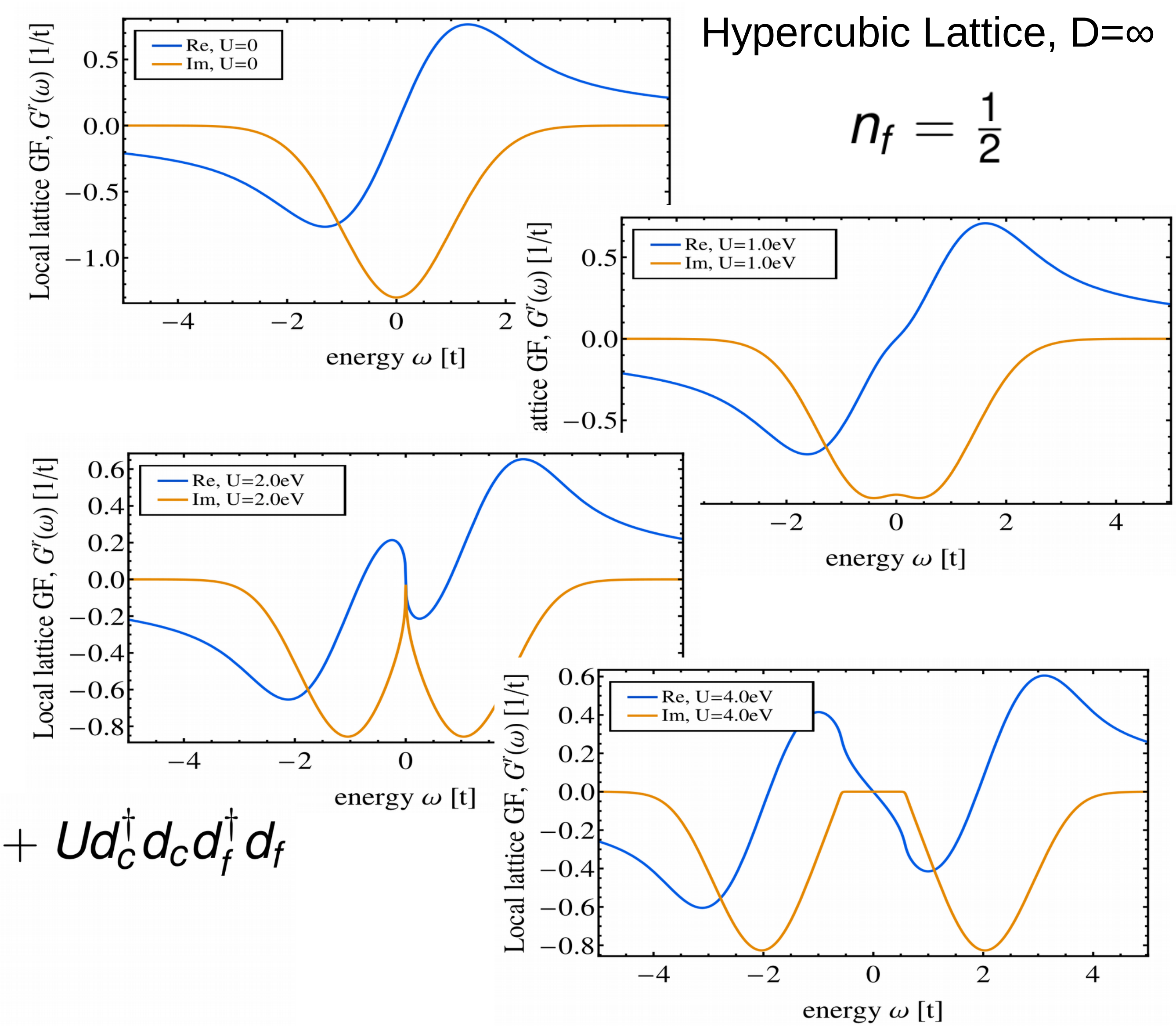
Okamoto, Mathey, RH, arXiv:1608.05399 (2016)

HQME as DMFT impurity solver



Hypercubic Lattice, D=∞

$$n_f = \frac{1}{2}$$



Falicov-Kimbal model

Test case, because
→ **exact** solution via **NEGF**
→ metal-insulator trans.

$$H_{\text{imp}} = \sum_{m\in\{c,f\}} \epsilon_m d_m^\dagger d_m + U d_c^\dagger d_c d_f^\dagger d_f$$

$$H_{\text{env}} = \sum_k \epsilon_k c_k^\dagger c_k$$

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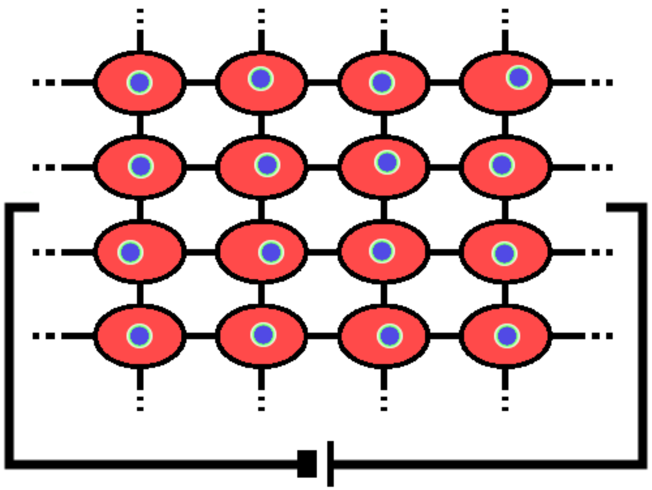
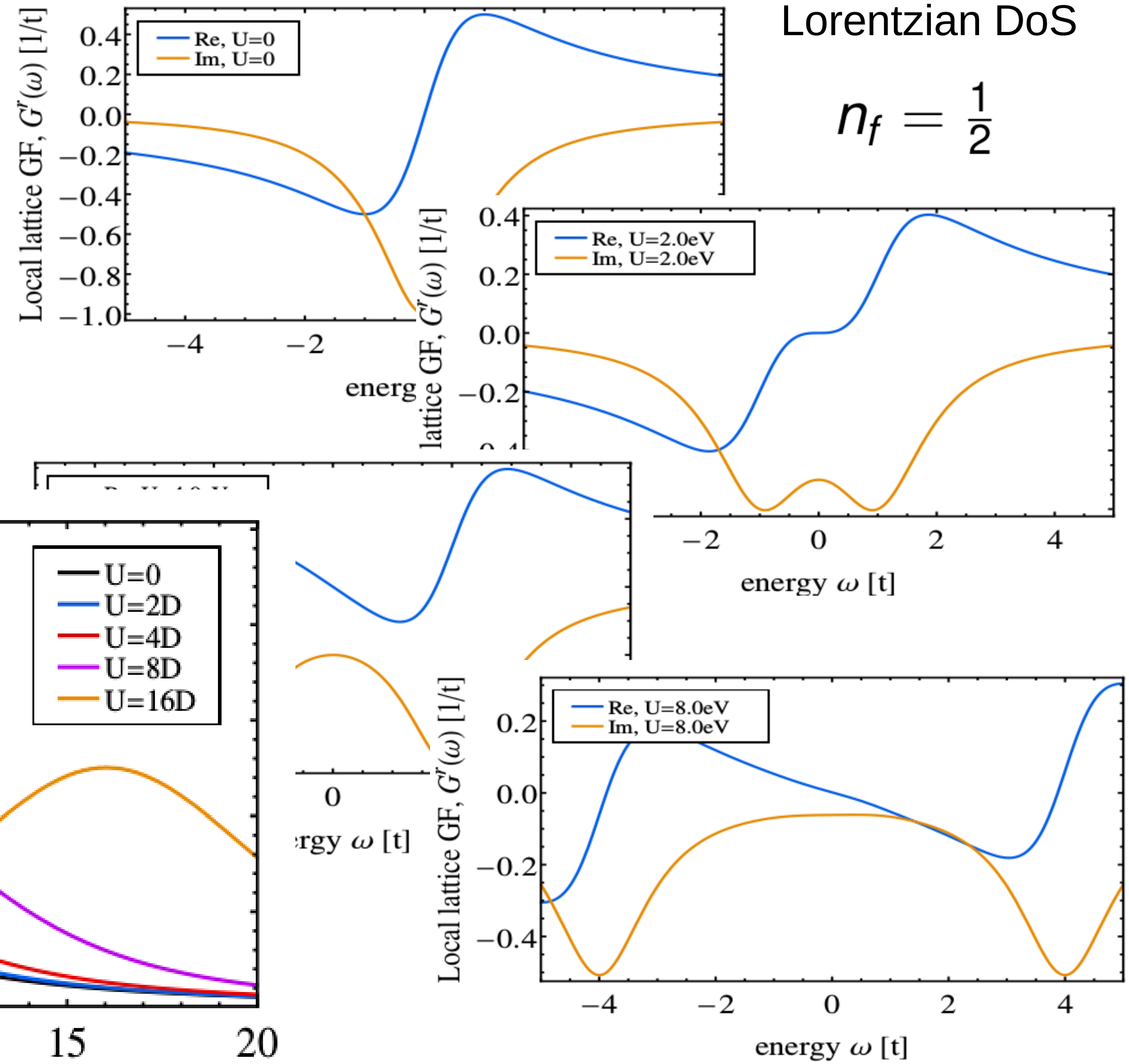
RH, Millis, to be developed (2016)

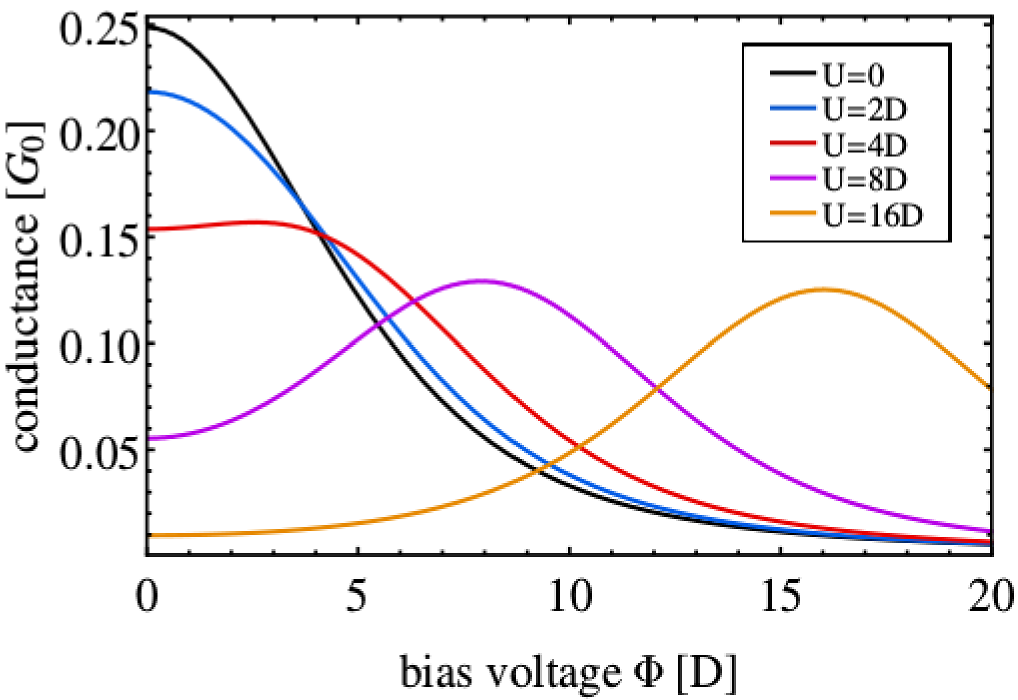


HQME as DMFT impurity solver

Lorentzian DoS

$$n_f = \frac{1}{2}$$

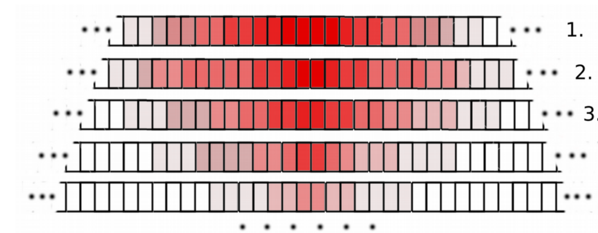




RH, Millis, to be developed (2016)

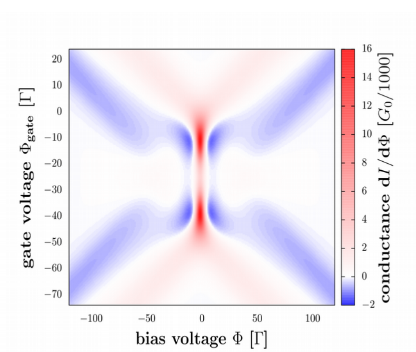
Summary and Outlook

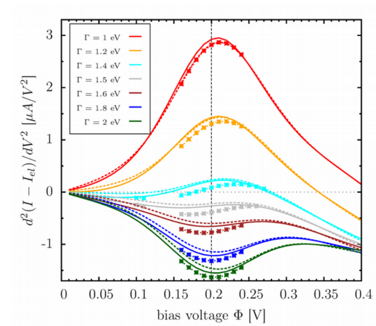
Characteristics of HQME
- based on hybridization expansion
- systematic truncation possible — see PRB 88, 235426 (2013)
- results are competible with CT-QMC — see PRB 92, 085430 (2015)
- time-local (access to long time scales)
- exact and perturbative results
- equilibrium and nonequilibrium dynamics
- any type of interactions
- polynomial scaling with complexity of the impurity (?)

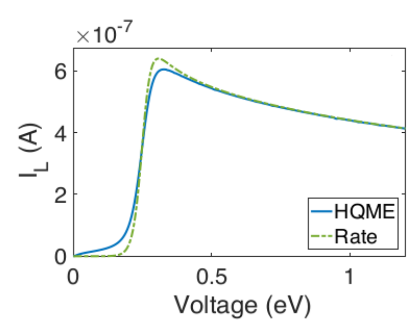


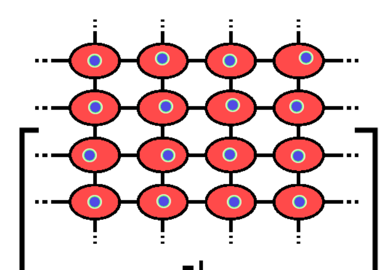
Extension to interacting environments / reservoirs
- impurity solver for DMFT applications (soon)
- transport with Luttinger liquid leads Okamoto, RH, arXiv:1608.05399 (2016)

Physics:









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