Quantum Impurity Models in and out of equilibrium studied by means of Variational Cluster Perturbation Theory

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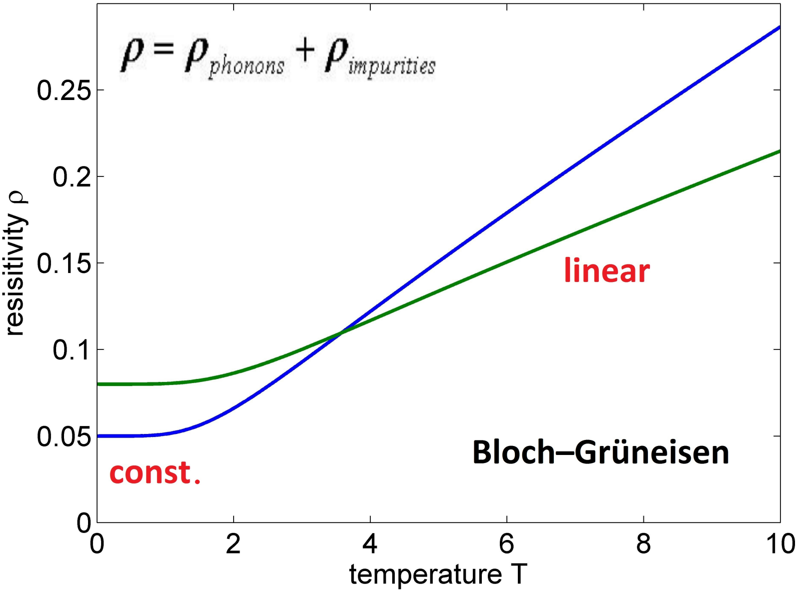
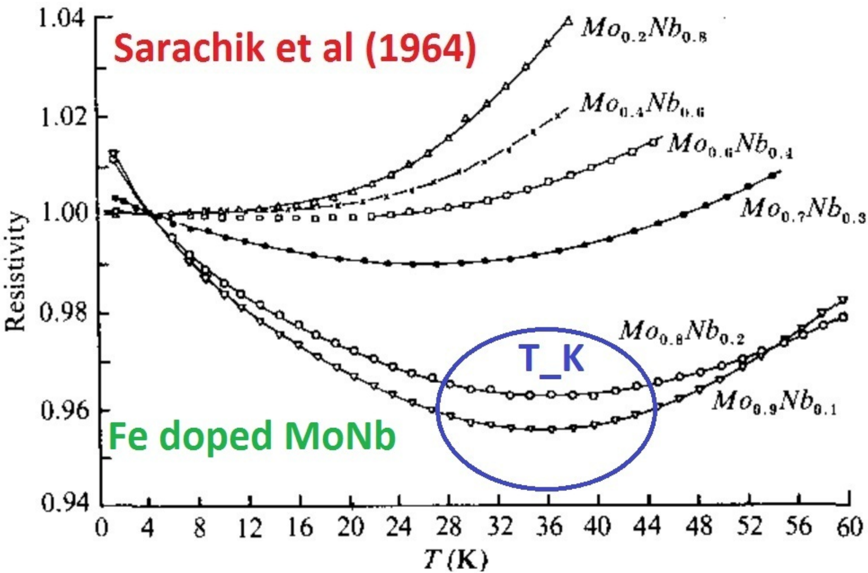
Quantum Impurity Problems

Resistivity in metals (I)

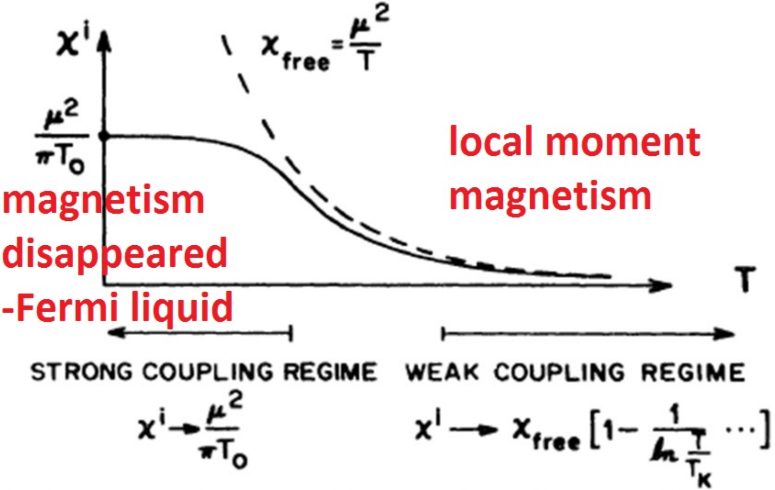


Resistivity in metals (II)



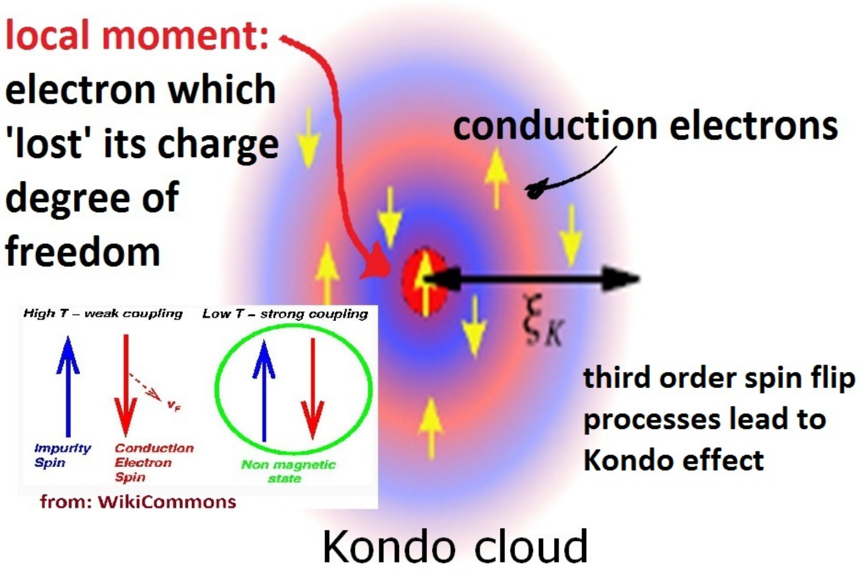
increased scattering at low T

What about susceptibility?

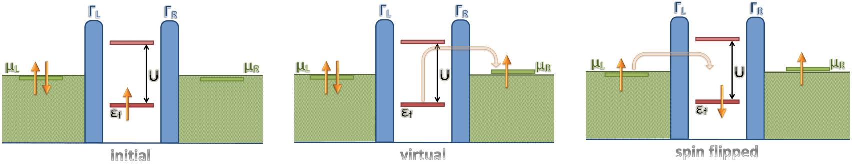


J.Mydosh: lecture notes on Kondo problem

Screening of local moments

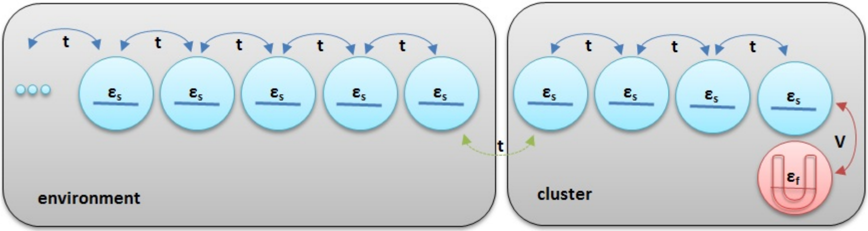


Quantum dot <-> Kondo physics, 1990's



- new experimental playground
- versatile
- tunable
- control over many parameters

Single Impurity Anderson Model - Cluster decomposition



Manybody Cluster Methods

Generic lattice model

$$\hat{\mathcal{H}} = \sum_{ij} t_{ij}\, c_i^\dagger\, c_j + \sum_{ijlk} U_{ijkl}\, c_i^\dagger\, c_j^\dagger\, c_k\, c_l$$
$$= \hat{\mathcal{H}}_I(t) + \hat{\mathcal{H}}_{II}(U)$$

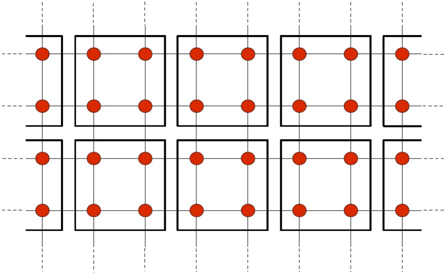
Perturbative methods

expand in some parameter:

- interaction (weak coupling)
- hopping (strong coupling)

Cluster Perturbation Theory[a] [b]

[a] C. Gros and R. Valenti, Phys. Rev. B 48, 418 (1993)
[b] D. Sénéchal, D. Perez, and M. Pioro-Ladriére, Phys. Rev. Lett. 84, 522 (2000)



Extrapolate cluster to thermodynamic limit:

$$\mathsf{G}^{-1}(\omega, \mathbf{k}) = \mathsf{G}_{\text{cluster}}{}^{-1}(\omega) - \mathsf{T}(\mathbf{k})$$

- G . . . lattice Green's function
- $\mathsf{G}_{\text{cluster}}$ . . . exact Green's function of the **cluster**
- T . . . **inter**-cluster off diagonal one particle terms (i.e. hopping)

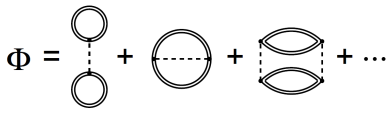
Variational Cluster Approach [a]

[a]M. Potthoff, M. Aichhorn, and C. Dahnken, Phys. Rev. Lett. 91, 206402 (2003)

- VCA = variational extension to CPT - rigorously developed within the **Self-Energy Functional Approach**[a b],
- **grand potential functional**:

$$\Omega[\Sigma, \mathsf{G}_0] = F[\Sigma] - \mathrm{Tr}\ln\left(-\mathsf{G}_0^{-1} + \Sigma\right).$$

- Luttinger-Ward functional $F[\Sigma]$ = sum of all **two-particle irreducible** diagrams



[a]M. Potthoff, Eur. Phys. J. B 32, 429 (2003)
[b]M. Potthoff, Eur. Phys. J. B 36, 335 (2003)

VCA Reference System (I)

same interaction part $\hat{\mathcal{H}}_{II}(U) \longrightarrow$ same $F[\Sigma]$

$$\hat{\mathcal{H}}' = \hat{\mathcal{H}}_I(t') + \hat{\mathcal{H}}_{II}(U)$$

- **same lattice**,
- **same interaction**,
- may have entirely different **single-particle** operators / **parameters**.

VCA Reference System (II)

The reference system $\hat{\mathcal{H}}'$ may be used to **eliminate the Luttinger-Ward functional**: (This is still exact!)

$$\begin{aligned} \Omega[\Sigma] &= F[\Sigma] - \mathsf{Tr}\left\{\ln\left(-\mathsf{G}_0^{-1} + \Sigma\right)\right\} \\ \Omega'[\Sigma] &= F[\Sigma] - \mathsf{Tr}\left\{\ln\left(-\mathsf{G}_0'^{-1} + \Sigma\right)\right\} \,|- \\ \hline \Omega[\Sigma] &= \Omega'[\Sigma] + \mathsf{Tr}\left\{\ln\left(-\mathsf{G}_0'^{-1} + \Sigma\right)\right\} - \mathsf{Tr}\left\{\ln\left(-\mathsf{G}_0^{-1} + \Sigma\right)\right\} \\ &= \Omega'[\Sigma] - \mathsf{Tr}\left\{\ln\left(-\mathsf{G}'[\Sigma]\right)\right\} + \mathsf{Tr}\left\{\ln\left(-\mathsf{G}[\Sigma]\right)\right\} \end{aligned}$$

Grand Potential Functional $\Omega[\Sigma]$

Dyson's equation is recovered at the stationary point of the grand potential functional $\Omega[\Sigma]$

$$\beta \frac{\delta F[\Sigma]}{\delta \Sigma} = -\mathsf{G}$$

$$\beta \frac{\delta \Omega[\Sigma, \mathsf{G}_0]}{\delta \Sigma} = -\mathsf{G} + \left(\mathsf{G}_0^{-1} - \Sigma\right)^{-1} \stackrel{!}{=} 0 \,.$$

VCA - Overview

- **Grand potential**

$$\Omega(t') = \Omega'(t') + \mathsf{Tr}\left\{\ln\left(-\mathsf{G}(t')\right)\right\} - \mathsf{Tr}\left\{\ln\left(-\mathsf{G}'(t')\right)\right\} \ .$$

- **Stationarity condition:**

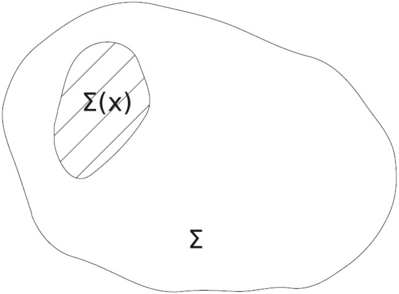
$$\nabla_{t'}\Omega(t') \stackrel{!}{=} 0 \ .$$

- **Green's function** of the physical system G

$$\mathsf{G}^{-1} = \mathsf{G}'^{-1} - \mathsf{T} \ .$$

Restriction of self-energies

The self-energy $\Sigma(t)$ is given by the self-energy of the reference system $\Sigma(t)$, where t denotes the single particle parameters, **restricting the space of available self-energies**.



Results in equilibrium

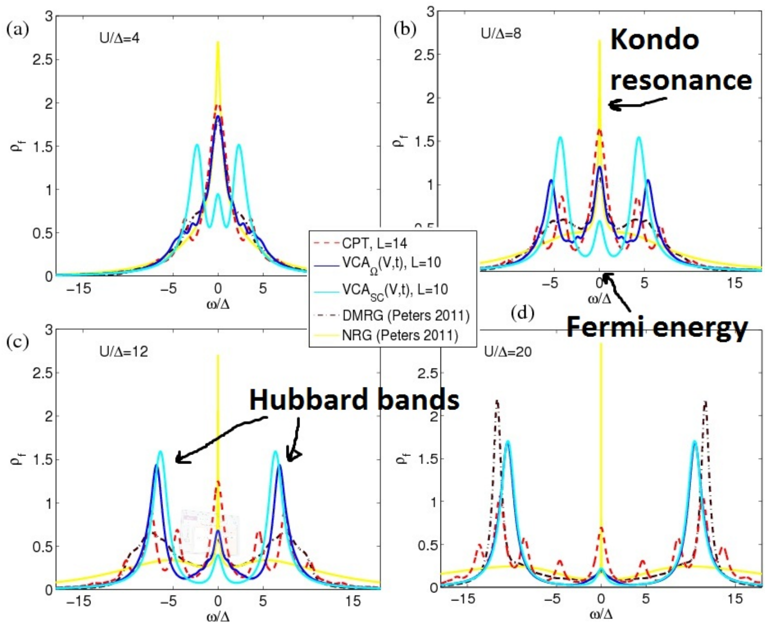
Spectral properties

- Local impurity density of states (single-particle spectral function):

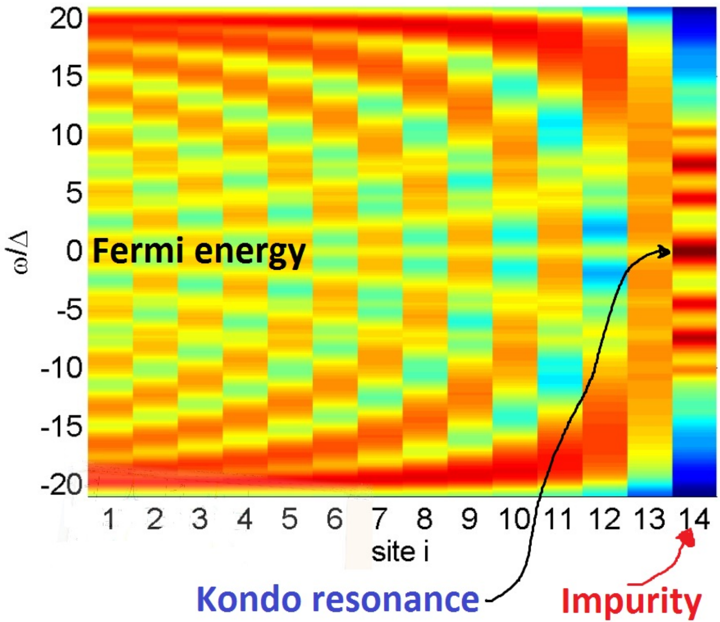
$$A_f^\sigma(\omega) = -\frac{1}{\pi}\,\mathrm{Im}\,\mathrm{G}_{ff}^{\sigma,\mathrm{ret}}(\omega)\ .$$

- Probability to find electronic states at a given energy ω.
- Fermi energy = 0

Spectral properties



Spectral properties (spatial)



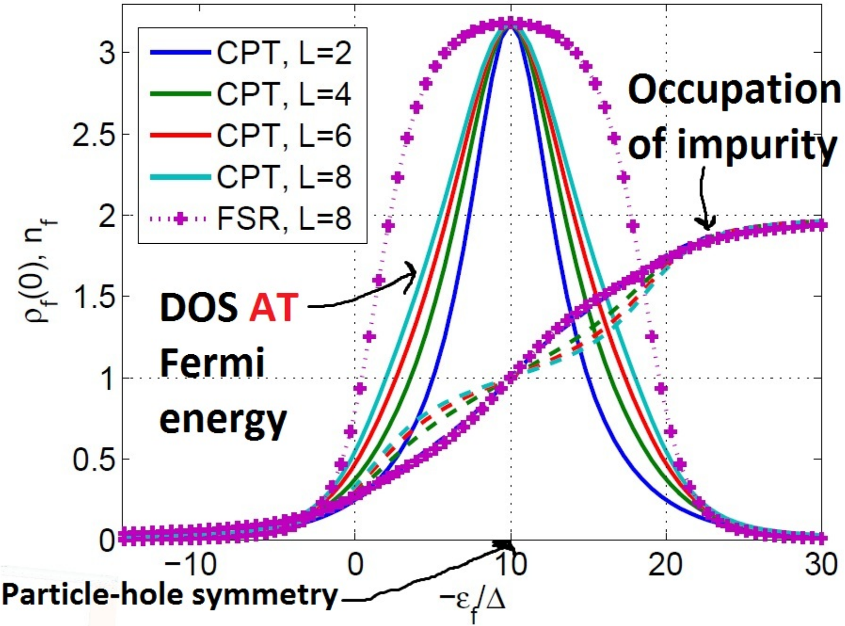
Impurity Occupation (I)

- The **Friedel sum rule** is "naturally" fulfilled within VCA_Ω where $\text{x} = \{\epsilon_s, \epsilon_f\}$:

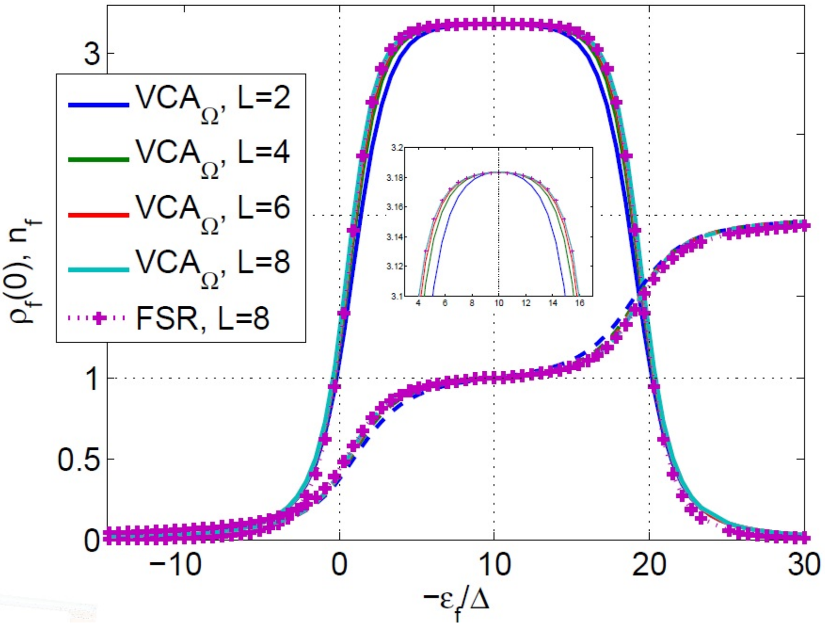
$$\rho_{f,\sigma}(0) = \frac{\sin^2\left(\pi < n_\sigma^f >\right)}{\pi\Delta} \quad .$$

- Local version of Luttinger theorem in Fermi liquid theory.

Impurity Occupation (II)



Impurity Occupation (III)



Kondo Temperature

- Since the height of the Kondo resonance is fixed by the Friedel sum rule, the **spectral weight** (area) of Kondo peak and it's **FWHM** are **proportional** to T_K.
- The Kondo temperature (symmetric SIAM) is given by **Bethe Ansatz**[2]

$$T_K = \sqrt{\frac{\Delta U}{2}}\, e^{-\gamma \frac{\pi}{8\Delta} U} \,, \quad \gamma = 1 \,.$$

- An analytic calculation for a two-site reference system yields for VCA_Ω

$$\gamma = 0.6511 \,.$$

[2] A. C. Hewson, The Kondo Problem to Heavy Fermions (Cambridge University Press, 1997)

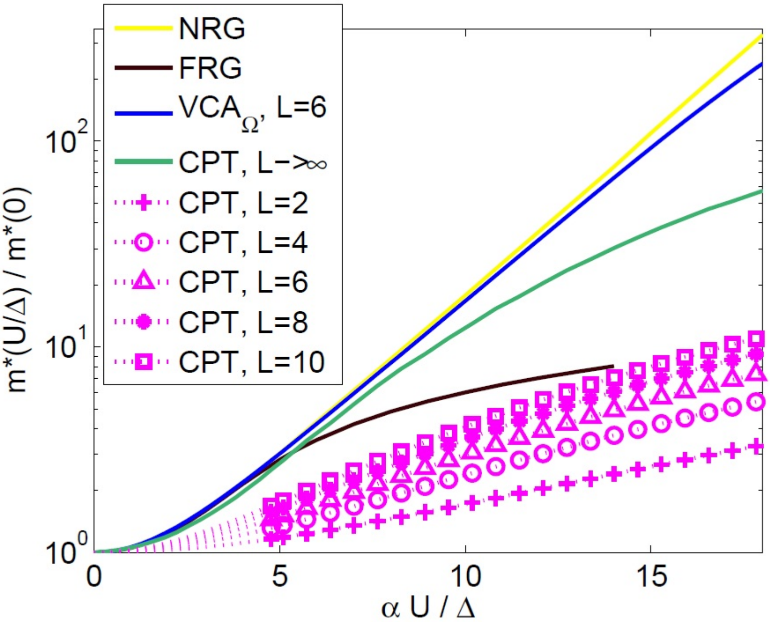
Effective Mass

- The **effective mass** (quasi-particle renormalization) is **inversely proportional** to the Kondo temperature[3]:

$$\frac{m^*(U)}{m^*(0)} = 1 - \left.\frac{d[\mathrm{Im}\,\Sigma^{\sigma}_{ff}(i\omega, U)]}{d\,\omega}\right|_{\omega=0^+}$$

[3] C. Karrasch, R. Hedden, R. Peters, T. Pruschke, K. Schönhammer, and V. Meden, J. Phys.: Condensed Matter 20, 345205 (2008)

Effective Mass

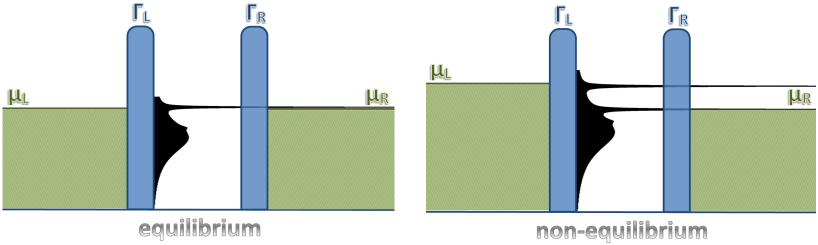


Conclusion

- **VCA** » CPT
- **Kondo peak** + exponential scale in U
- **Hubbard bands** (position + width)
- **all parameter regions** (pinning of Kondo resonance)
- Σ exact for high Matsubara frequency
- extension to **many orbitals**, **arbitrary dimensions**, **non-equilibrium** feasible
- **fast**

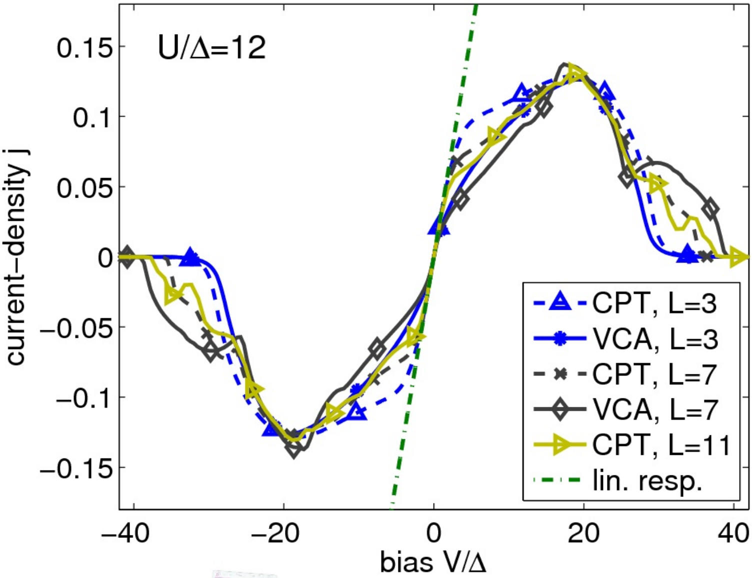
Results in a non-equilibrium situation

Nonequilibrium extension of VCA



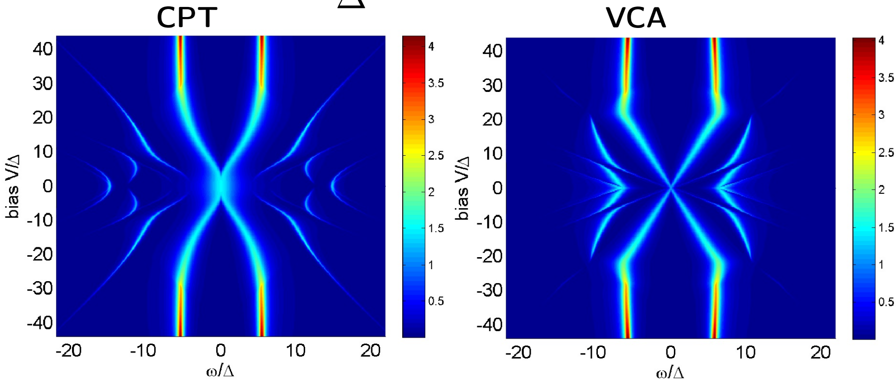
- **requires CPT/VCA reformulation for Keldysh Green's functions**
- Initial state: **three decoupled systems in equilibrium**
- At some time t_0 the **coupling is switched on**.
- We are interested in the long time **steady-state properties**.

Current for a single impurity orbital



Non-equilibrium density of states

$$\frac{U}{\Delta} = 12$$



Thank You!

Thank you for your attention!

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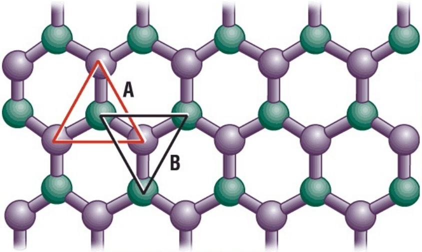
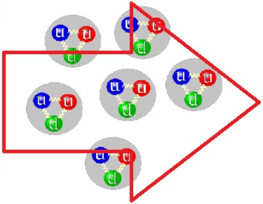
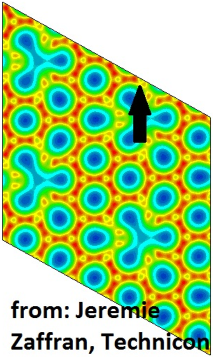
Magnetic vacancies in Graphene



from: ELECTROIQ





- Proton irradiation $\longrightarrow$ vacancies
- these behave like local moments and exhibit a Kondo effect
- effect of disorder
- **requires CPT/VCA extension by means of Green's function averaging**

Density of states for a given vacancy concentration