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

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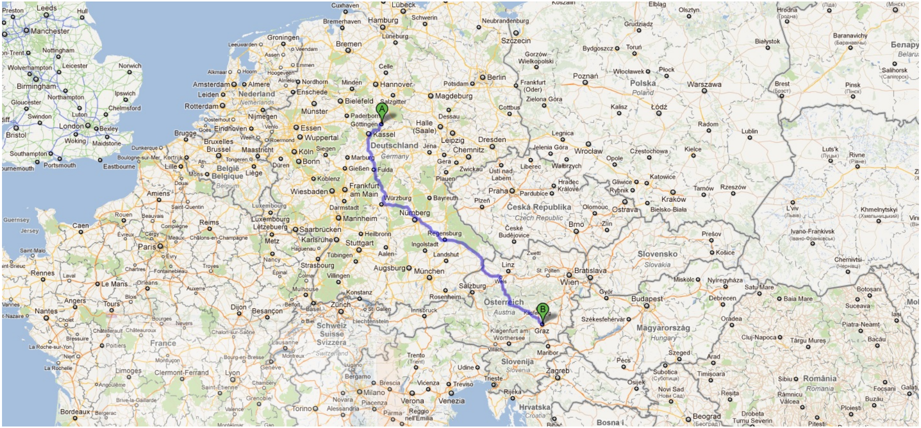
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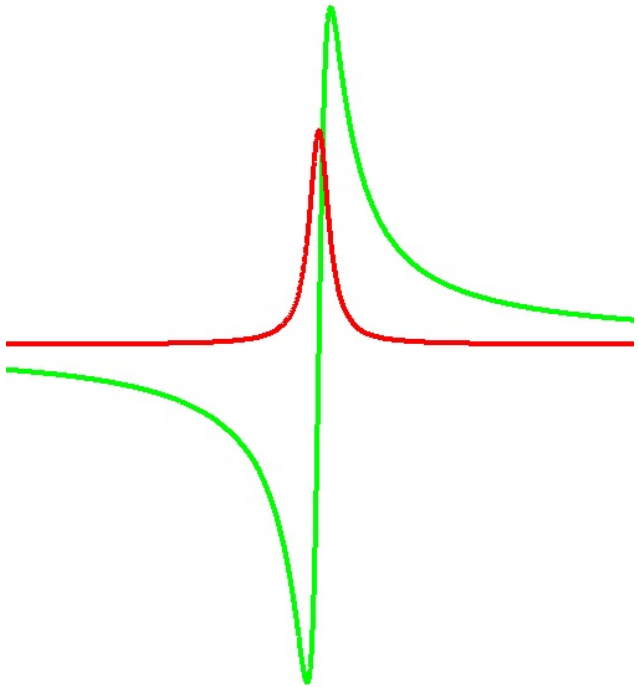
Generic lattice model

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

To apply a perturbative method one has to expand in some parameter. Usually the hopping (strong coupling) or the interaction (weak coupling) are considered.

Atomic limit

$$G(z;t,U) = \left\langle \frac{1}{z - \hat{\mathcal{H}}(t,U)} \right\rangle$$

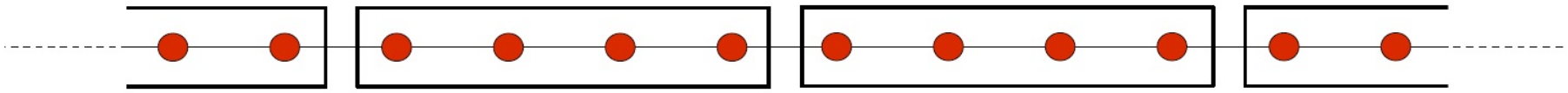


- strong coupling perturbation theory (in hopping t)
- consider $G(t=0)$ as starting point

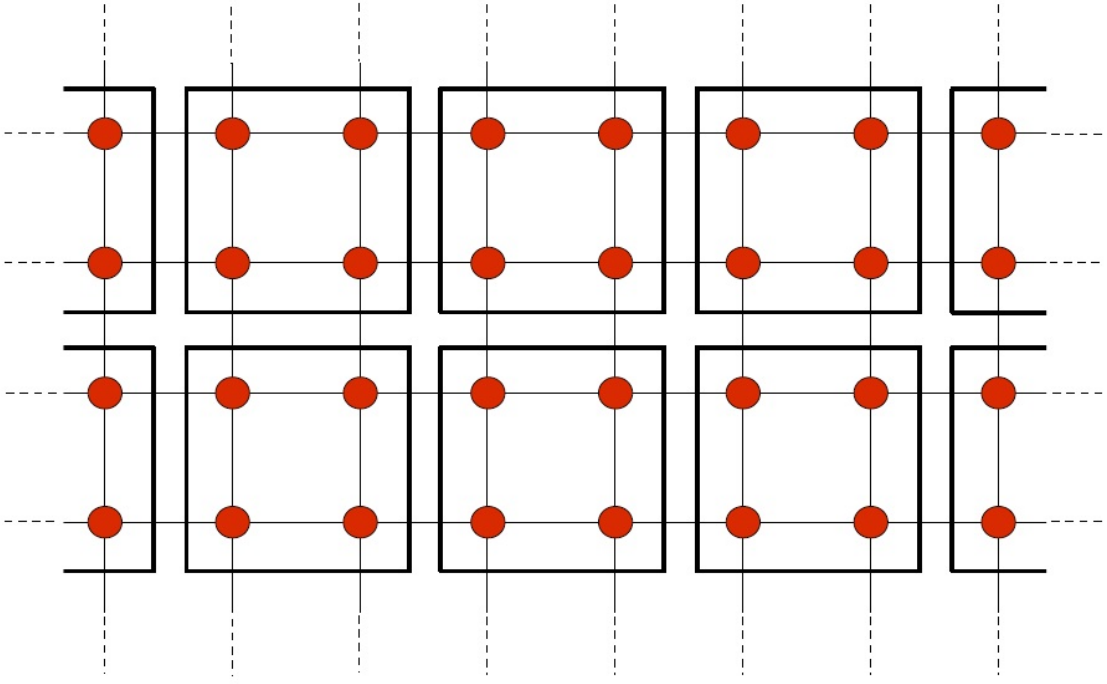
Cluster decompositions of lattice models

Taking this idea one step further - introducing a superlattice τ:
lattice γ = superlattice τ + cluster

one dimensional chain



two dimensional square lattice



$$\mathbf{r} = \tilde{\mathbf{r}} + \mathbf{R}$$

$$\mathbf{k} = \tilde{\mathbf{k}} + \mathbf{K}$$

$\mathbf{r} \in \gamma$, $\mathbf{R} \in$ cluster, $\tilde{\mathbf{r}} \in \tau$

$\mathbf{k} \in \mathrm{BZ}_\gamma$, $\mathbf{K} \in \mathrm{BZ}_\tau$,

$\tilde{\mathbf{k}} \in \mathrm{BZ}_\gamma \cap$ rec. superlattice

Manybody Cluster Methods

- Cluster Perturbation Theory (**CPT**)
- Variational Cluster Perturbation Theory (**VCPT**)
  (= Variational Cluster Approach (**VCA**))
- Cluster/Cellular Dynamical Mean-Field Theory (**CDMFT**)
- Dynamical Cluster Approximation (**DCA**) (momentum space CDMFT)

CPT and VCA may be developed within the Self-Energy Functional Approach (**SFA**)[a b].

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

Cluster Perturbation Theory[a] [b]

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

By means of strong coupling perturbation theory it can be shown that the first order result for the lattice Green function G is

$$\mathsf{G}^{-1}(\omega, \mathbf{k}) = \mathsf{G}'^{-1}(\omega) - \mathsf{T}(\mathbf{k})$$

- G' is the exact Green's function of the **cluster**
- Tcontains just the **inter**-cluster off diagonal one particle terms (i.e. hopping)

Cluster Perturbation Theory (II)

Heuristic derivation using **Dyson's equation**:

$$G^{-1} = G_0^{-1} - \Sigma$$
$$G'^{-1} = G_0'^{-1} - \Sigma$$

- G' is the exact Green's function **of the cluster**, $_0$ denotes non-interacting Green's functions
- Σ is the self-energy

$$G_0^{-1} = \omega + \mu - V$$

- V is the hopping matrix of the full problem

Cluster Perturbation Theory (III)

$$
\begin{aligned}
G^{-1} &= G_0^{-1} - \Sigma \\
&\approx G_0^{-1} - \Sigma' \\
&= G_0^{-1} - \left(G_0'^{-1} - G'^{-1}\right) \\
&= G'^{-1} - \left(G_0'^{-1} - G_0^{-1}\right) \\
&= G'^{-1} - T
\end{aligned}
$$

- Approximation made: take for the self-energy the **self-energy of the cluster**
- T is defined as the inter-cluster hopping:

$$
\begin{aligned}
\left(G_0'^{-1} - G_0^{-1}\right) &= \left(\omega + \mu - V'\right) - \left(\omega + \mu - V\right) \\
&= V - V' = T
\end{aligned}
$$

Cluster Perturbation Theory - Requirements

CPT enables you to calculate an approximation to the Green's function of the full system given:

1. The **exact solution** of the cluster Green's function. (Which is usually obtained by exact diagonalization (Band-Lanczos).)
2. The **inter-cluster hopping matrix** $\mathbf{T_{rr'}}$. In most cases a partial Fourier transform in superlattice wavevectors

$$\mathbf{T_{RR'}}(\tilde{\mathbf{k}}) = \sum_{\tilde{\mathbf{r}} \in \tau} e^{i\,\tilde{\mathbf{k}}\cdot\tilde{\mathbf{r}}}\, \mathbf{T_{rr'}} \text{ where } \begin{cases} \mathbf{r} = & \mathbf{R} \\ \mathbf{r'} = & \tilde{\mathbf{r}} + \mathbf{R'} \end{cases}$$

is needed. This depends solely on the single particle hopping matrix and on the lattice geometry.

Cluster Perturbation Theory - Limits

- Since CPT is derived from strong coupling perturbation theory it is exact in the limit $\frac{U}{t} \to \infty$. (Here U may be a homogeneous on-site repulsion, and t a uniform nearest-neighbor hopping.)
- In the case $U \to 0$ self-energy vanishes and consequently CPT is also exact in that limit.
- CPT is exact in the limit $L \to \infty$, where L is the size of the cluster.
- The CPT formula of the Green's function is the lowest order result of strong coupling perturbation theory. Nevertheless results are not improved by considering higher order expansion terms but rather by considering larger clusters.
- The cluster is usually solved exactly. Therefore CPT captures short-range correlations exactly while long-range correlations are treated perturbatively.

Variational Cluster Approach[a]

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

- VCA may be seen as a variational extension to CPT - rigorously developed within the Self-Energy Functional Theory.(SFT)
- VCA does **not** implement a variational principle in the sense of a Rayleigh-Ritz variational principle where an upper bound to the groundstate is obtained. Neither are variational wave functions in use.

Grand Potential Ω (I)

The grand potential Ω may be expressed as a functional of the Green's function

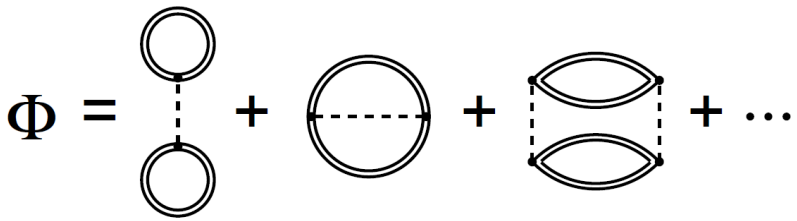
$$\Omega[\mathrm{G}] = \Phi[\mathrm{G}] - \mathrm{Tr}\left\{\left(\mathrm{G}_0^{-1} - \mathrm{G}^{-1}\right)\mathrm{G}\right\} + \mathrm{Tr}\left\{\ln\left(-\mathrm{G}\right)\right\}$$

$$\mathrm{Tr} = \frac{1}{\beta N}\sum_{\tilde{\omega}_n} e^{i\tilde{\omega}_n 0^+}\,\mathrm{tr}\ ,\ \mathrm{tr} = \sum\ (\text{lattice sites, spin, ...})\ ,\ i\tilde{\omega}_n\ = \frac{i\,2\pi n}{\beta}$$

The Luttinger-Ward Functional is denoted by $\Phi[\mathrm{G}]$, N is the number of lattice sites and β the inverse temperature. (Note that functions are understood in a matrix-function sense since G is a matrix in site/spin space.)

Luttinger-Ward functional $\Phi[G]$

- $\Phi[\Omega]$ = sum of all two-particle irreducible diagrams



- The functional derivative of $\Phi[G]$ is the self-energy:

$$\frac{\delta\Phi[G]}{\delta G} = \Sigma$$

- It is a **universal functional** of G in the following sense: whatever the form of the one-body Hamiltonian, it depends on the interaction only. This is one of the most important properties in order to obtain VCA.

Grand Potential Ω (II)

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

$$\begin{aligned}\frac{\delta\Omega[G]}{\delta G} &= \frac{\delta\Phi[G]}{\delta G} - \frac{\mathrm{Tr}\left\{\left(G_0^{-1} - G^{-1}\right)G\right\}}{\delta G} + \frac{\mathrm{Tr}\left\{\ln\left(-G\right)\right\}}{\delta G} \\ &= \Sigma - G_0^{-1} + G^{-1} \stackrel{!}{=} 0 \\ &\Rightarrow G^{-1} = G_0^{-1} - \Sigma\end{aligned}$$

- Factors of βN are omitted here.

Grand Potential Ω (III)

- This is a **dynamic variational principle** since it involves $G(\omega)$ (excited states are involved).
- At the stationary point (**and only there**) the grand potential functional $\Omega[G]$ is equal to the physical grand potential Ω. (And G to the physical Green's function.)

Legendre Transform of $\Omega[G]$ (IV)

It can be shown that

$$\frac{\delta \Phi[G]}{\delta G} = \Sigma \,,$$

is locally invertible. Therefore we may rewrite $\Omega[G]$ as $\Omega[G[\Sigma]]$:

$$\Omega[\Sigma] = F[\Sigma] - \mathrm{Tr}\left\{\left(-G_0^{-1} + \Sigma\right)\right\}$$
$$F[\Sigma] = \Phi[\Sigma] - \mathrm{Tr}\left\{\Sigma G\right\} \,,$$

again

$$\frac{\delta F[\Sigma]}{\delta \Sigma} = -G$$
$$\frac{\delta \Omega[\Sigma]}{\delta \Sigma} = -G + \left(G_0^{-1} - \Sigma\right)^{-1} \stackrel{!}{=} 0 \,.$$

VCA approximation

We are still left with the problem of evaluating the Luttinger-Ward functional, which in general is impossible. There exist three different suggestions for approximations:

- **Type I** Derive the Euler equation $\frac{\delta\Omega[\Sigma]}{\delta\Sigma} = 0$ and then choose (a physically motivated) **simplification of the equation** afterwards to render the determination of Σ possible.
- **Type II** Approximate $\Phi[G]$ by a **finite set of diagrams**.
- **Type III Restrict the domain** of allowed Σ's. This is what VCA is doing.

VCA Reference System (I)

Since systems which share the same interaction part $\hat{\mathcal{H}}_{II}(U)$ have the same $\Phi[G]$ (or $F[\Sigma]$) we construct a **reference system**:

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

- defined on the **same lattice**,
- having the **same interaction** as the original system,
- but may have entirely different **single-particle** operators / **parameters**.

VCA Reference System (II)

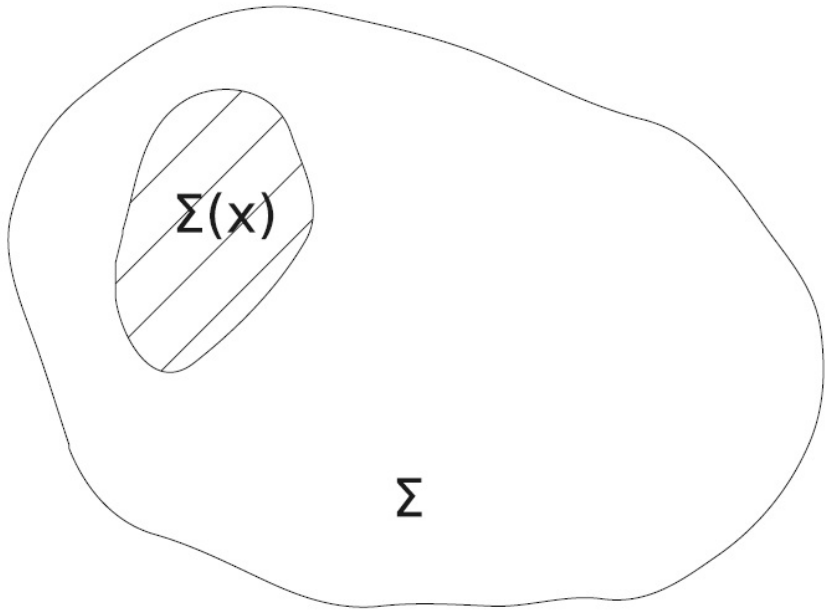
The reference system $\hat{\mathcal{H}}'$ may be used to **eliminate the Luttinger-Ward functional**: (This is still exact!)

$$\Omega[\Sigma] = F[\Sigma] - \mathrm{Tr}\left\{\ln\left(-G_0^{-1} + \Sigma\right)\right\}$$
$$\Omega'[\Sigma] = F[\Sigma] - \mathrm{Tr}\left\{\ln\left(-G_0'^{-1} + \Sigma\right)\right\}$$
$$-\sum$$
$$\begin{aligned}\Omega[\Sigma] &= \Omega'[\Sigma] + \mathrm{Tr}\left\{\ln\left(-G_0'^{-1} + \Sigma\right)\right\} - \mathrm{Tr}\left\{\ln\left(-G_0^{-1} + \Sigma\right)\right\} \\ &= \Omega'[\Sigma] + \mathrm{Tr}\left\{\ln\left(-G'[\Sigma]\right)\right\} - \mathrm{Tr}\left\{\ln\left(-G[\Sigma]\right)\right\}\end{aligned}$$

The signs in front of the term involving G and G' depend on the bosonic/fermionic case (just interchanged). (Shown are the bosonic signs.)

Evaluation of the grand potential (I)

Adopting a **Type-III approximation** we approximate the self-energy $\Sigma(x)$ by the self-energy of the reference system $\Sigma(x')$, where x denotes the single particle parameters, limiting the space of available self-energies.



VCA - Overview (I)

- The expression for the **grand potential** (for fermions) hereby becomes

$$\Omega(x') = \Omega'(x') + \mathrm{Tr}\left\{\ln\left(-G(x')\right)\right\} - \mathrm{Tr}\left\{\ln\left(-G'(x')\right)\right\} \ .$$

- The **stationarity condition** determining the physical parameters is then given by

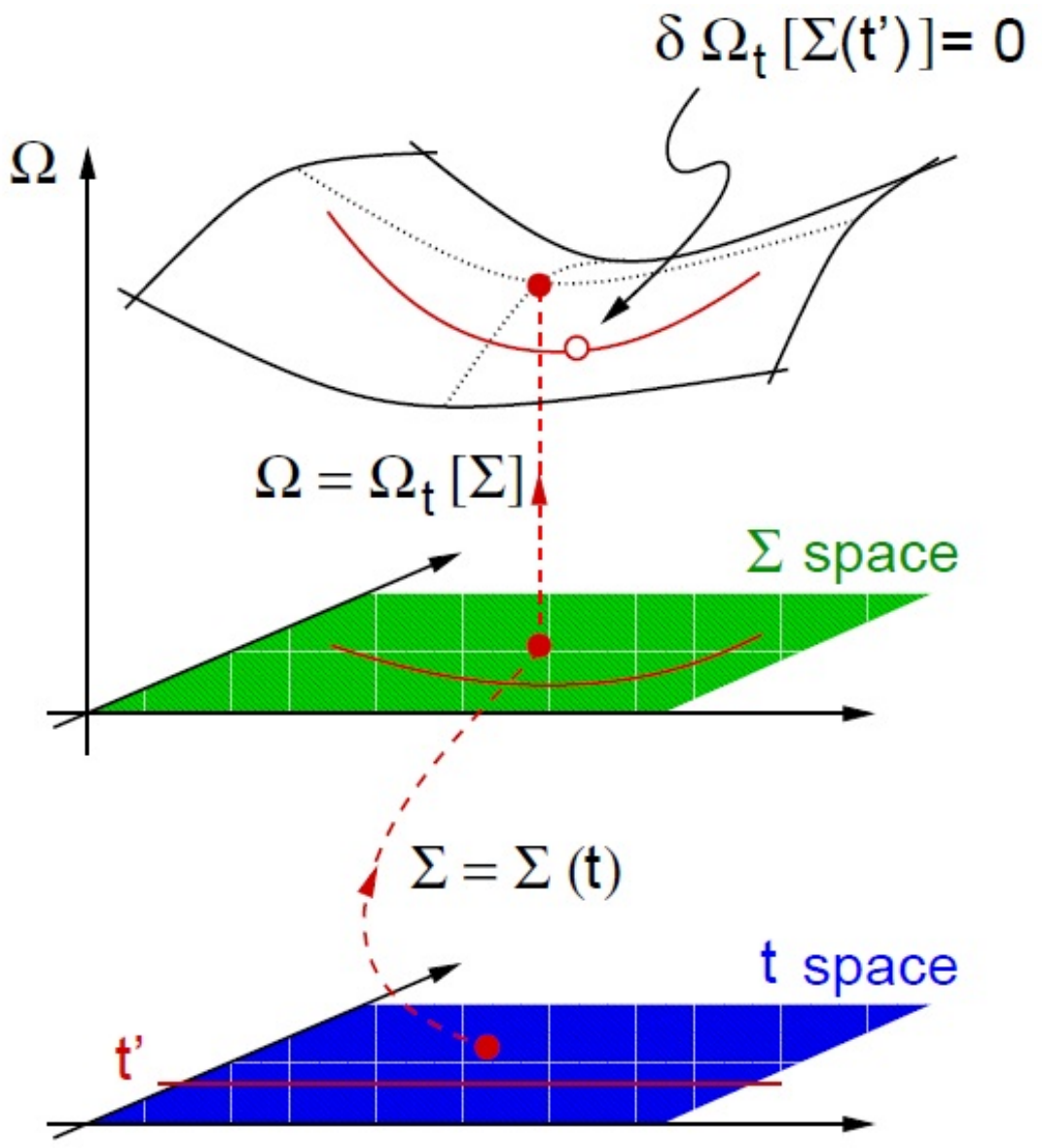
$$\nabla_{x'}\Omega(x') \stackrel{!}{=} 0 \ .$$

- The **Green's function** of the physical system G is obtained in CPT/VCA by Dyson's equation

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

The matrix $T = G_0'^{-1} - G_0^{-1}$ contains all single particle terms not included in the reference system (as in CPT) as well as the deviation, introduced by VCA, $\Delta x \equiv x' - x$ of the single-particle parameters of the reference system x' with respect to the ones of the original system x.

VCA - Overview (II)



from: M. Potthoff, arXiv/1108.2183 (2010)

VCA - History

- In the past VCA was successfully applied to **fermionic** as well as **bosonic** models[2].
- VCA was extended to deal with systems with **broken-symmetry phases** (like models in ferromagnetic, superfluid, or superconducting phase)[345].
- CPT/VCA is applicable for systems at **finite temperature**[6].
- It may be applied to **disordered systems**[7].
- Recently CPT/VCA were extended to deal with **nonequilibrium problems**[89].

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[2] W. Koller and N. Dupuis, J. Phys.: Condens. Matter 18, 9525 (2006)

[3] C. Dahnken, M. Aichhorn, W. Hanke, E. Arrigoni, and M. Potthoff, Phys. Rev. B 70, 245110 (2004)

[4] M. Knap, E. Arrigoni, W. von der Linden, arXiv.org/1010.4295 (2010)

[5] E. Arrigoni, M. Knap, W. von der Linden, arXiv.org/1103.3664 (2011)

[6] M. Aichhorn, M. Daghofer, H. G. Evertz, and W. von der Linden, Phys. Rev. B 67, 161103(R) (2003)

[7] M. Knap, E. Arrigoni, and W. von der Linden , Phys. Rev. A 82, 053628 (2010)

[8] M. Balzer, M. Potthoff, arXiv/1102.3344

[9] M. Knap, W. von der Linden, E. Arrigoni, arXiv.org/1104.3838

VCA - Advantages

- comparatively **fast**,
- **flexible** to any model, geometry, dimensionality, ... ,
- **controlled** approximation within size of the reference system,
- **single particle dynamic quantities** as well as **static expectations values** are directly accessible via G(z),
- the Green's function is available in Matsubara as well as in **real frequency**

Review Articles

On cluster methods (CPT, VCA, CDMFT,...):

D.Sénéchal, arXiv.org/0806.2690 (2008)

On SFT:

M. Potthoff, arXiv/1108.2183 (2010)

Piled Higher and Deeper ***by Jorge Cham*** **www.phdcomics.com**

Seminar BINGO!

To play, simply print out this bingo sheet and attend a departmental seminar.

Mark over each square that occurs throughout the course of the lecture.

The first one to form a straight line (or all four corners) must yell out BINGO!! to win!

SEMINAR BINGO

Speaker bashes previous work	Repeated use of "um…"	Speaker sucks up to host professor	Host Professor falls asleep	Speaker wastes 5 minutes explaining outline
Laptop malfunction	Work ties in to Cancer/HIV or War on Terror	"…et al."	You're the only one in your lab that bothered to show up	Blatant typo
Entire slide filled with equations	"The data *clearly* shows…"	FREE Speaker runs out of time	Use of Powerpoint template with blue background	References Advisor (past or present)
There's a Grad Student wearing same clothes as yesterday	Bitter Post-doc asks question	"That's an interesting question"	"Beyond the scope of this work"	Master's student bobs head fighting sleep
Speaker forgets to thank collaborators	Cell phone goes off	You've no idea what's going on	"Future work will…"	Results conveniently show improvement

Single Impurity Anderson Model

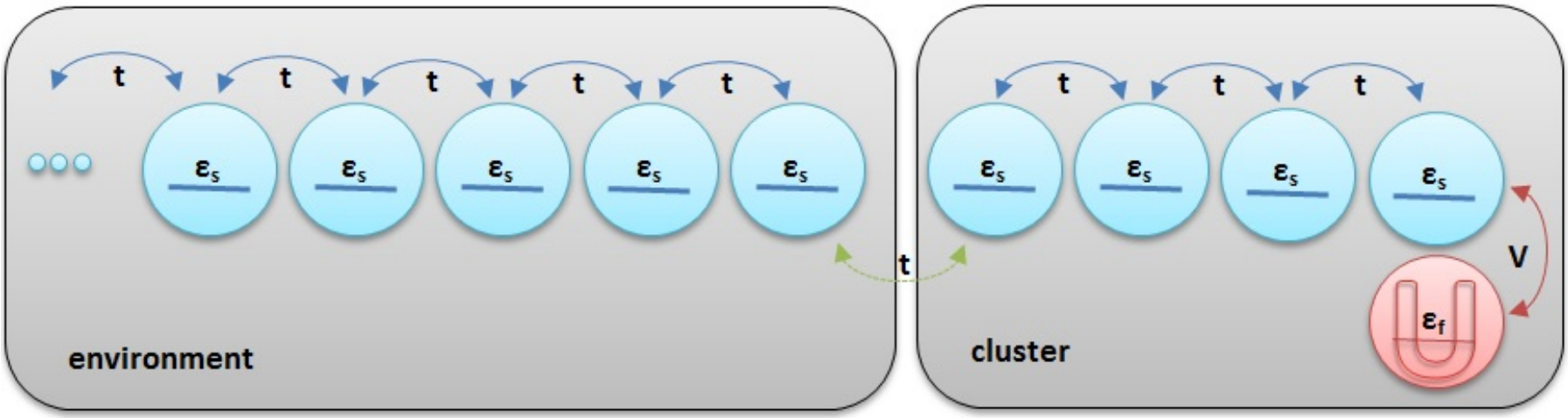
$$\hat{\mathcal{H}}_{\text{SIAM}} = \hat{\mathcal{H}}_{\text{conduction}} + \hat{\mathcal{H}}_{\text{impurity}} + \hat{\mathcal{H}}_{\text{hybridization}}$$

$$\hat{\mathcal{H}}^{L}_{\text{conduction}} = \epsilon_s \sum_{i}^{L} \sum_{\sigma} c^{\dagger}_{i\sigma} c_{i\sigma} - t \sum_{\langle i,j \rangle \sigma} c^{\dagger}_{i\sigma} c_{j\sigma}$$

$$\hat{\mathcal{H}}_{\text{impurity}} = \epsilon_f \sum_{\sigma} f^{\dagger}_{\sigma} f_{\sigma} + U \hat{n}^{f}_{\uparrow} \hat{n}^{f}_{\downarrow}$$

$$\hat{\mathcal{H}}_{\text{hybridization}} = -V \sum_{\sigma} c^{\dagger}_{l\sigma} f_{\sigma} + f^{\dagger}_{\sigma} c_{l\sigma}$$

Cluster decomposition



Grand potential for infinite reference systems

The reference system here consists of **two parts**:

- a cluster part and
- an infinite environment.

It is possible to find a **regular expression for the grand potential** (at zero temperature):

$$\Omega - \Omega'_{0,\text{env}} = \Omega'_{0,\text{cluster}} + \text{tr}\left\{\mathsf{T}\right\} - \frac{1}{\pi}\sum_{\sigma}\int_0^{\infty} d\omega \ln\left|\det\left(\mathbb{1}_{cc} - \tilde{\Sigma}_{cc}(i\omega)\mathsf{G}'_{cc}(i\omega)\right)\right| .$$

Numerical implementation

The Green's function of the reference system are obtained by

- Lanczos/Band-Lanczos method for the cluster part,
- analytically for the environment part.

Finding the stationary point of the grand potential is numerically challenging because it may be a minimum, a maximum or generally a saddle point and the dimensionality of the parameter space grows rapidly.

Results in equilibrium

Results

- **Spectral properties** (comparison to NRG, FRG[a], DMRG[b], CTQMC),
- Impurity **density of states and occupation** (Friedel sum rule) (comparison to Hubbard-X operator technique results[c], "Crossover" diagram (comparison to mean field results[d]))
- **Low energy properties**, Kondo temperature , effective mass, static spin susceptibility

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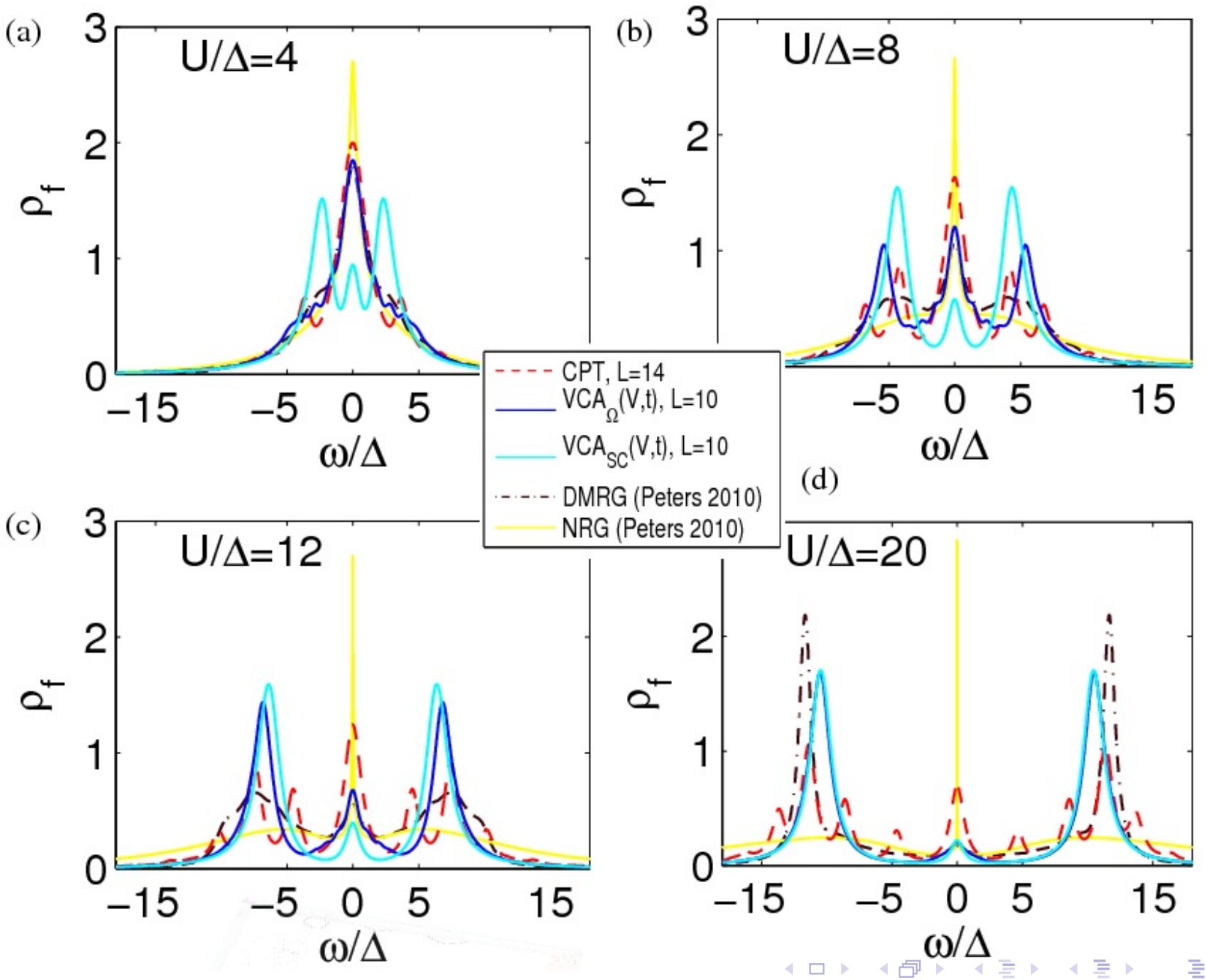
[a] C. Karrasch, R. Hedden, R. Peters, T. Pruschke, K. Schönhammer, and V. Meden, J. Phys.: Condensed Matter 20, 345205 (2008)

[b] R. Peters, 1103.5837 (2011)

[c] T. Lobo, M. S. Figueira, and M. E. Foglio, Nanotechnology 21, 274007 (2010)

[d] P. Coleman, AIP Conference Proceedings 629, 79 (2002)

Spectral properties



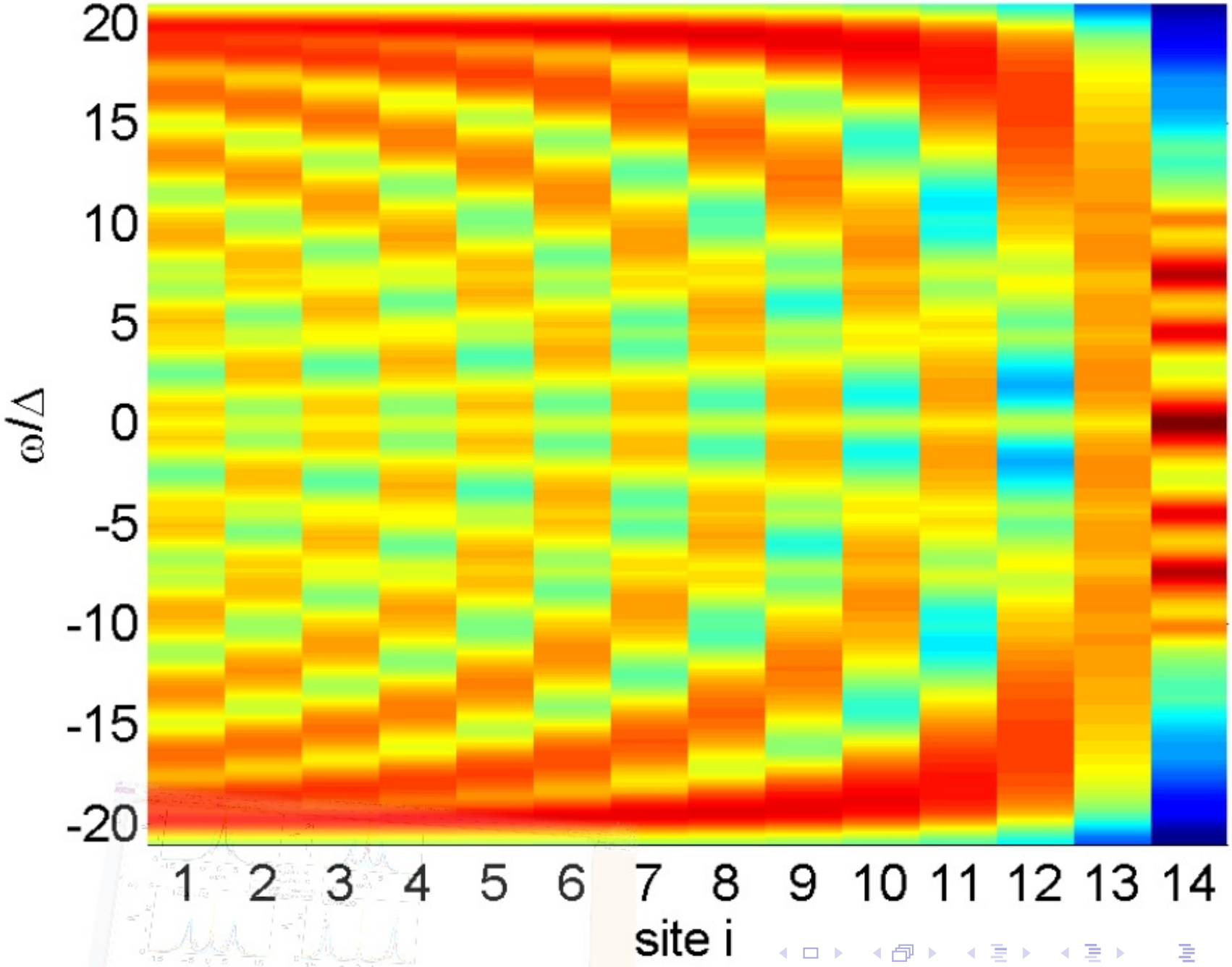
Spectral properties

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

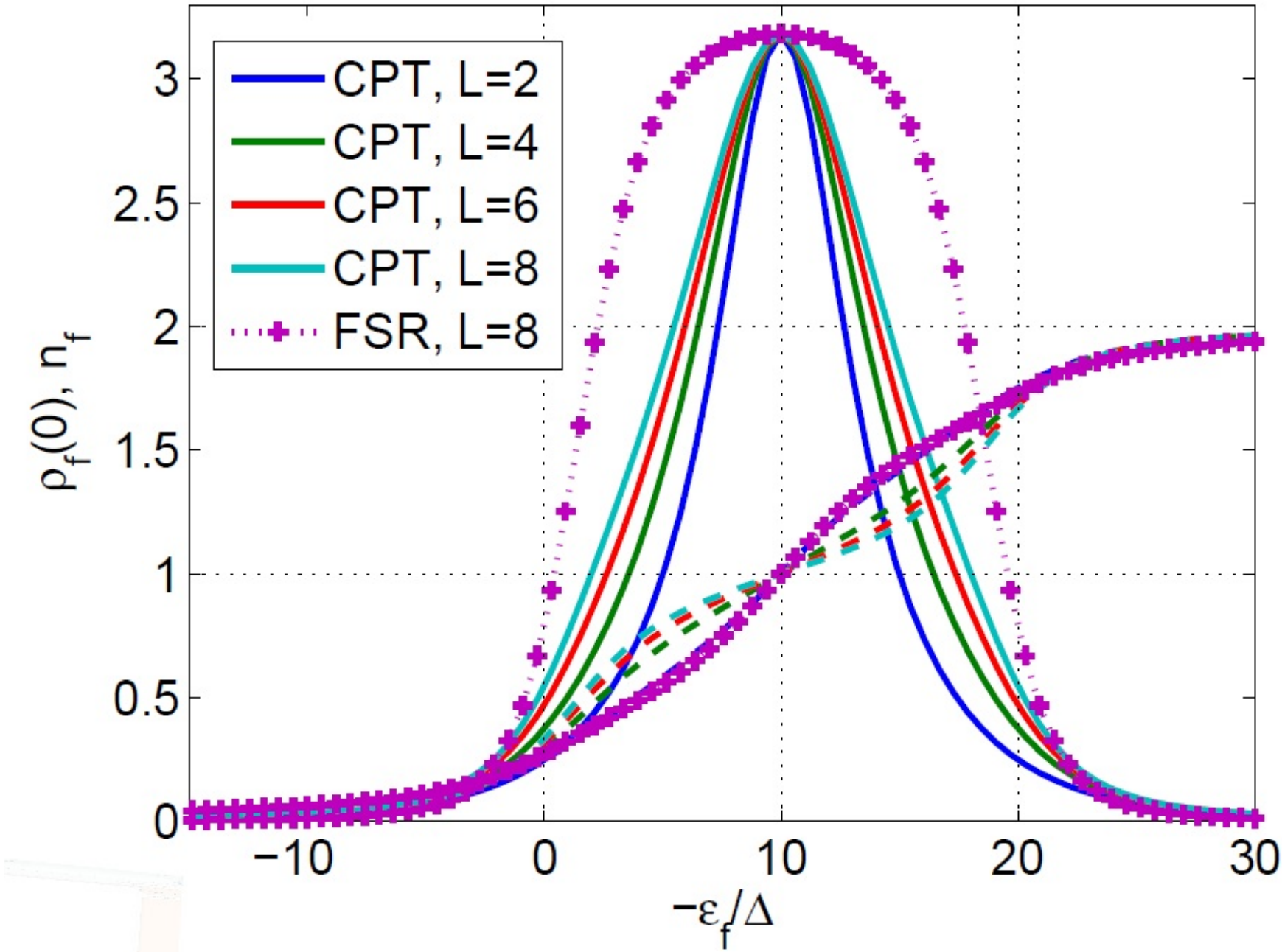
$$A_f^\sigma(\omega) = -\frac{1}{\pi} \operatorname{Im} \mathrm{G}_{ff}^{\sigma,\mathrm{ret}}(\omega) \ .$$

- Kondo peak reproduced, although with to much **weight** (looks even more exaggerated in figure because of large numerical broadening 0^+)
- Spurious finite size effects in **Hubbard bands** are almost eliminated by transitioning from CPT to VCA.
- VCA results (especially in low energy region) agree very well with (50 site) DMRG results.

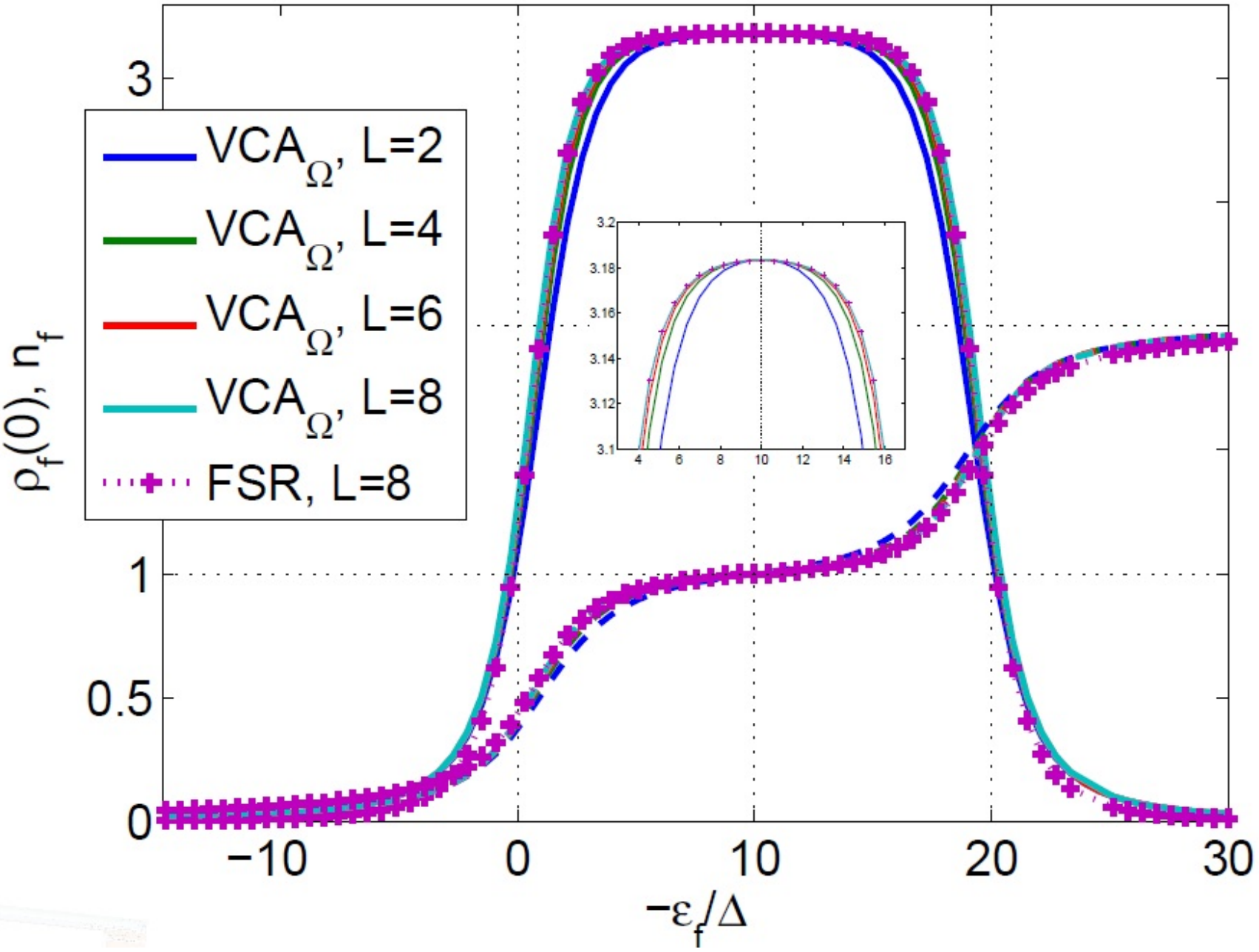
Spectral properties (spatial)



Impurity Occupation



Impurity Occupation

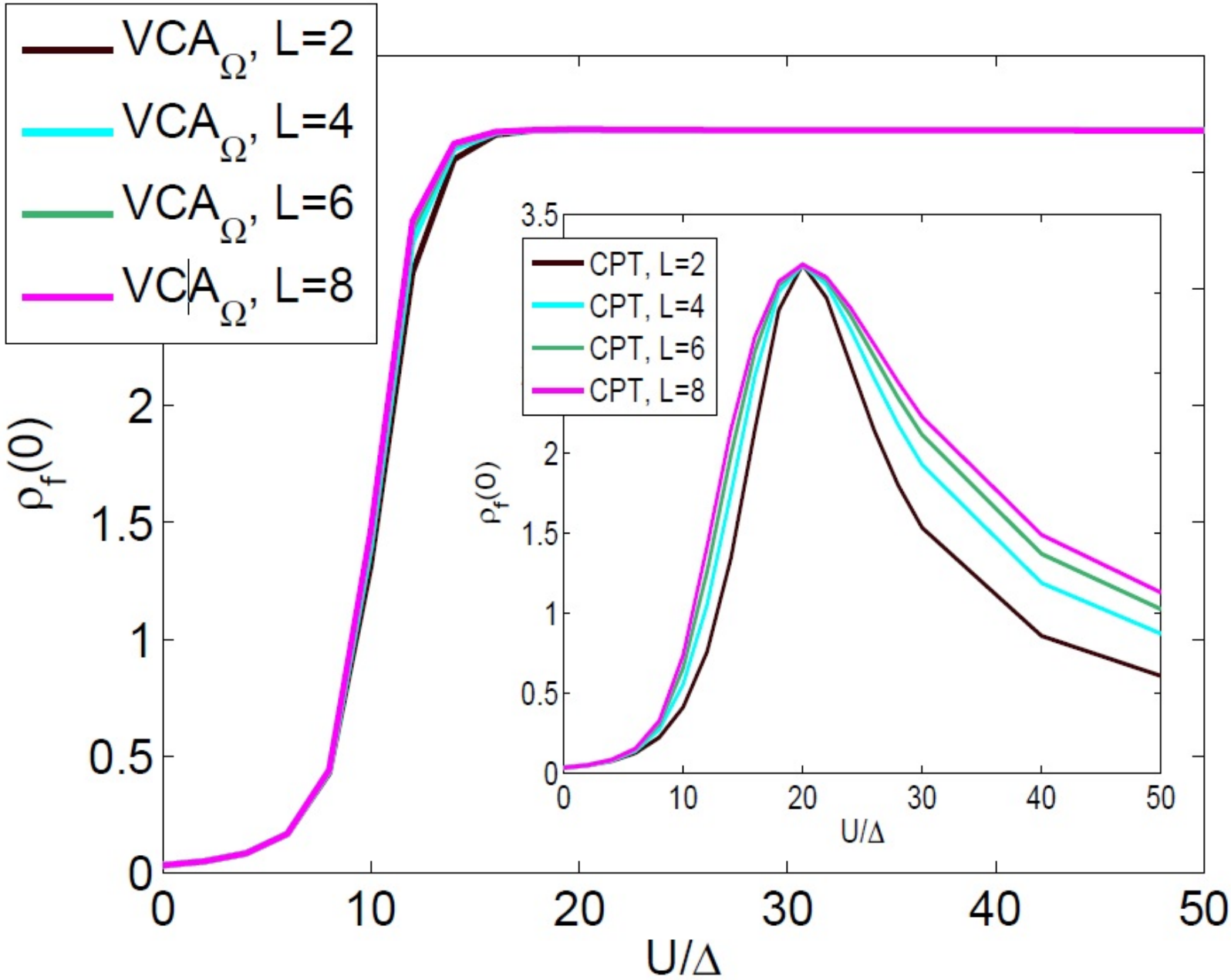


Impurity Occupation

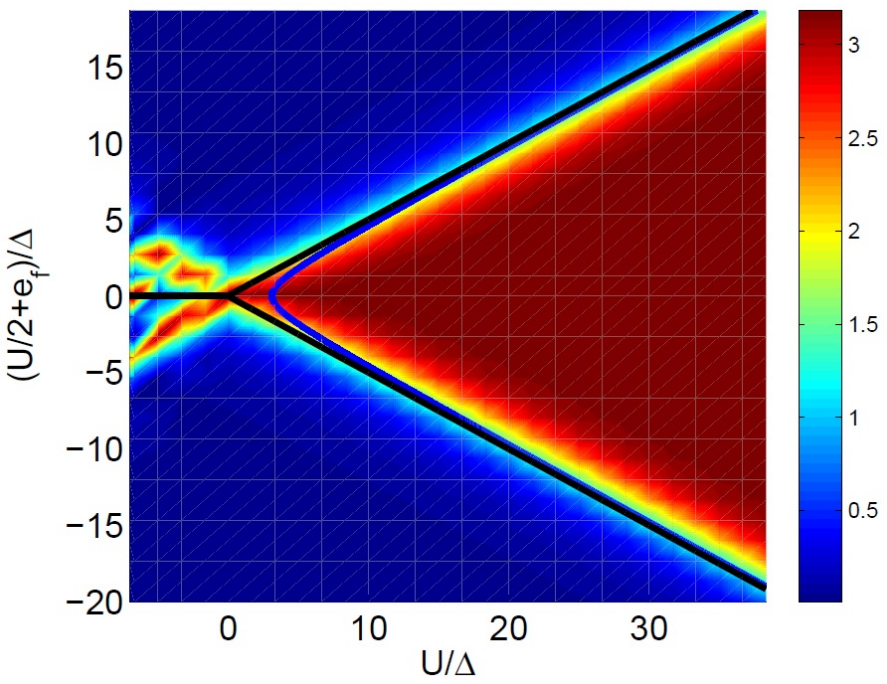
- CPT results slowly converge with increasing cluster size.
- VCA shows **rapid convergence** within very small sizes of the cluster part of the reference system. VCA reproduces the pinning of the Kondo peak remarkably well.
- The **Friedel sum rule** is "naturally" fulfilled within VCA_Ω where $\mathrm{x} = \{\epsilon_s, \epsilon_f\}$:

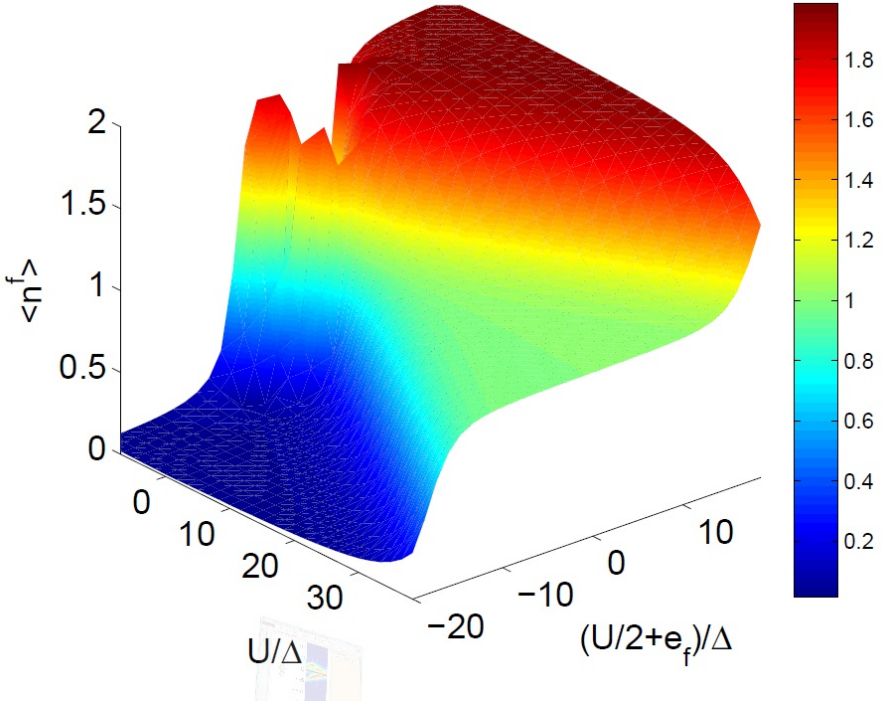
$$\rho_{f,\sigma}(0) = \frac{\sin^2\left(\pi < n_\sigma^f >\right)}{\pi\Delta} \quad .$$

Spectral Height of Kondo peak as function of the interaction

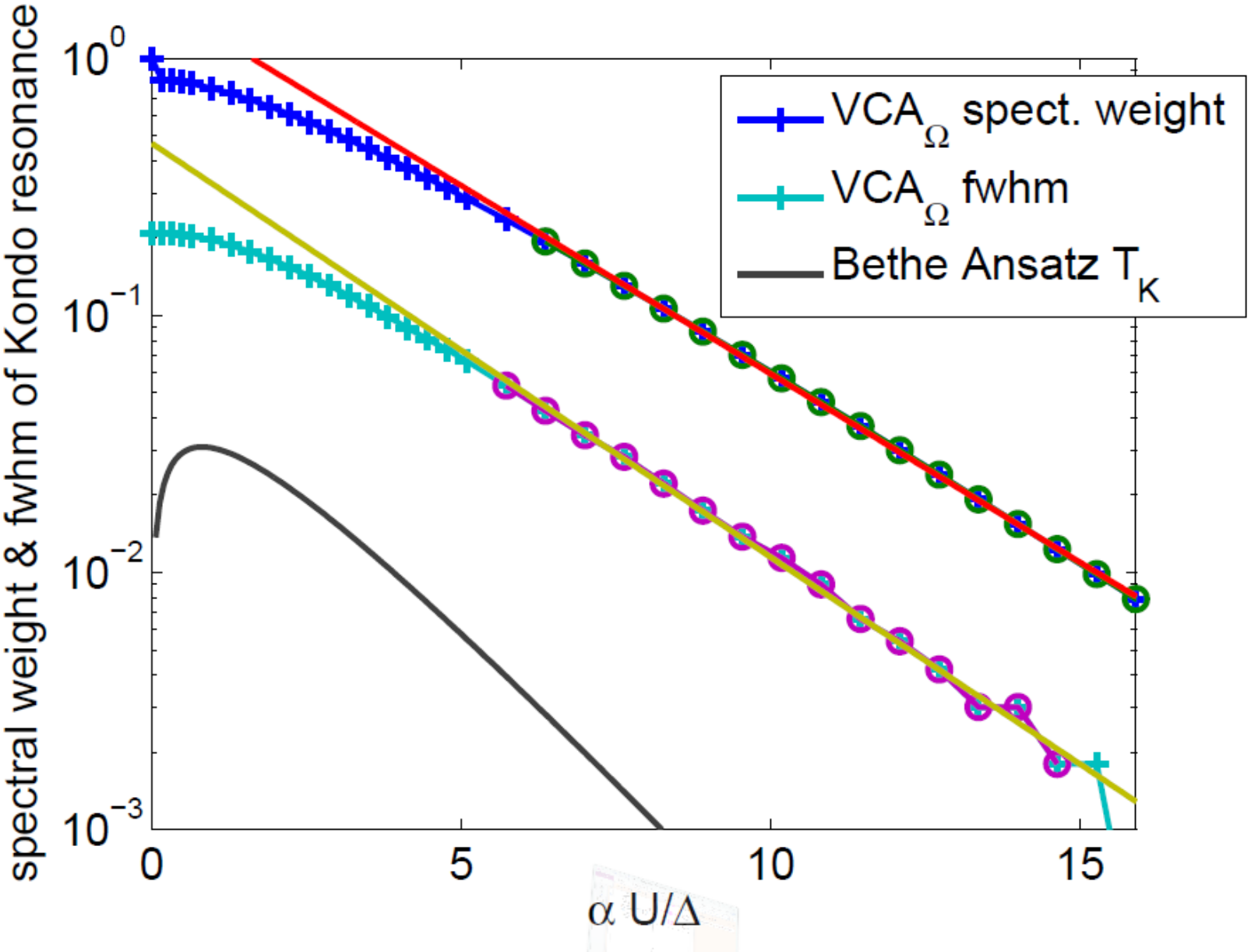


"Crossover" diagram





Kondo Temperature



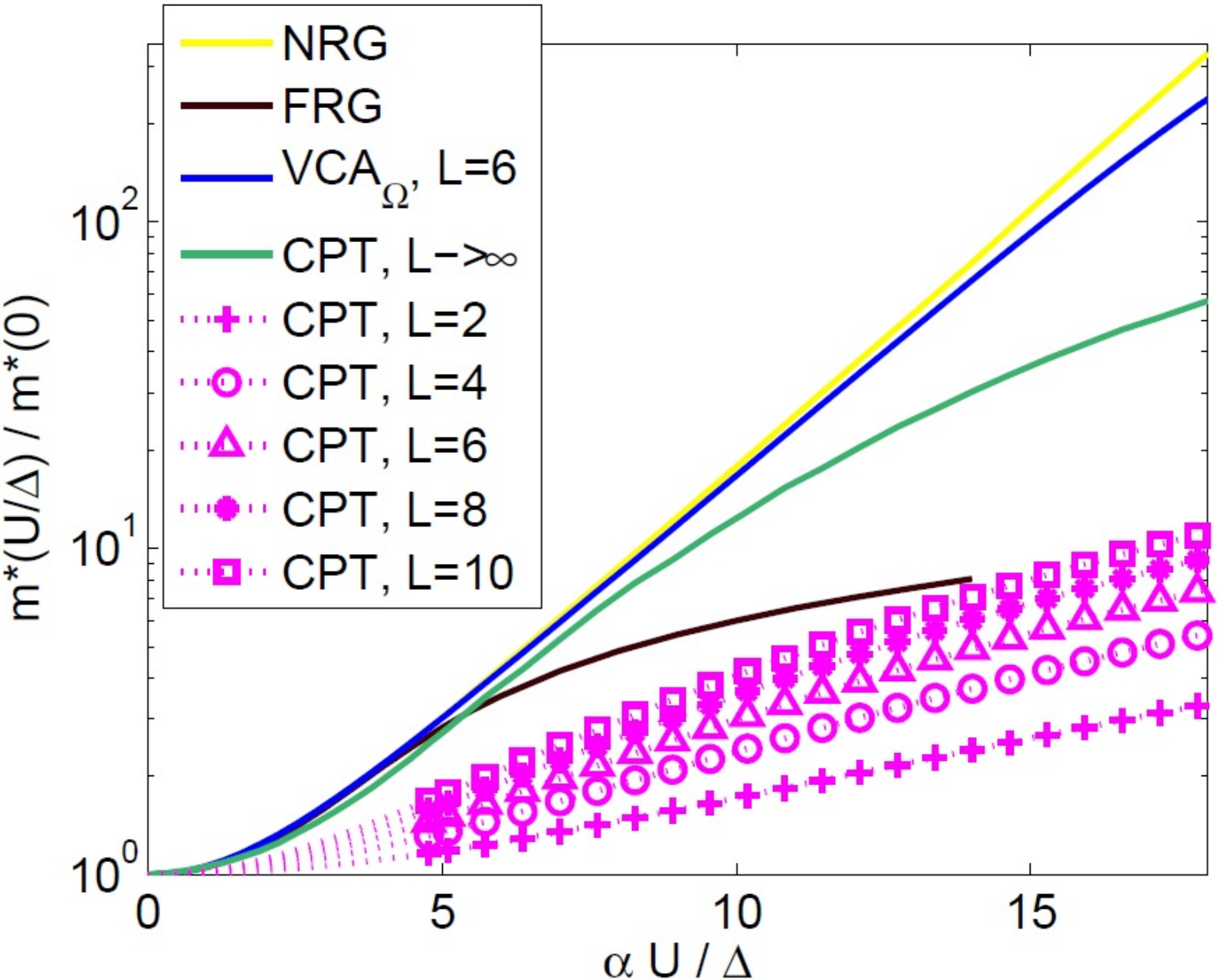
Kondo Temperature

- 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**[10]

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

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

Effective Mass



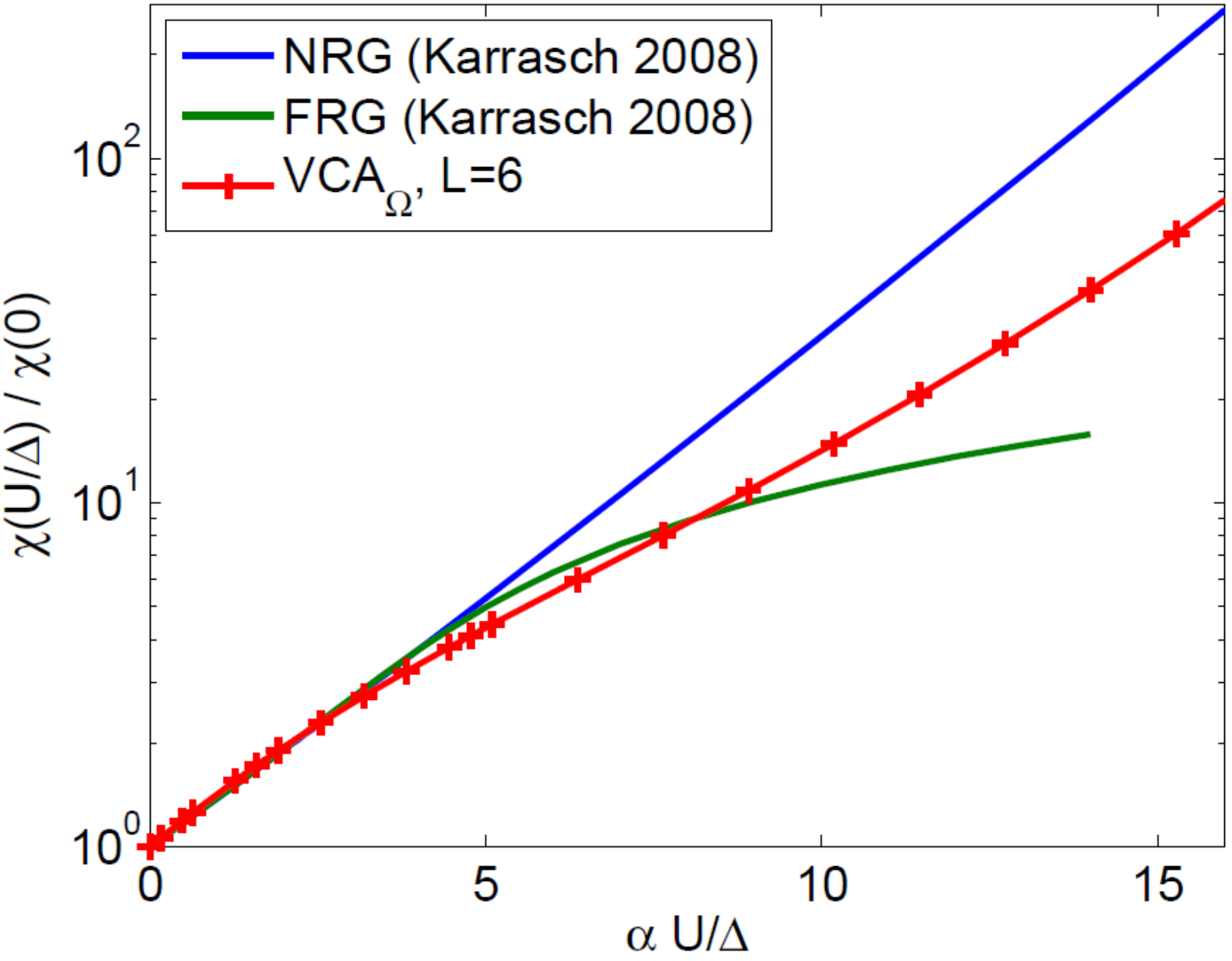
Effective Mass

- The **effective mass** (quasiparticle renormalization) is **inversely proportional** to the Kondo temperature[11]:

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

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

Static spin susceptibility

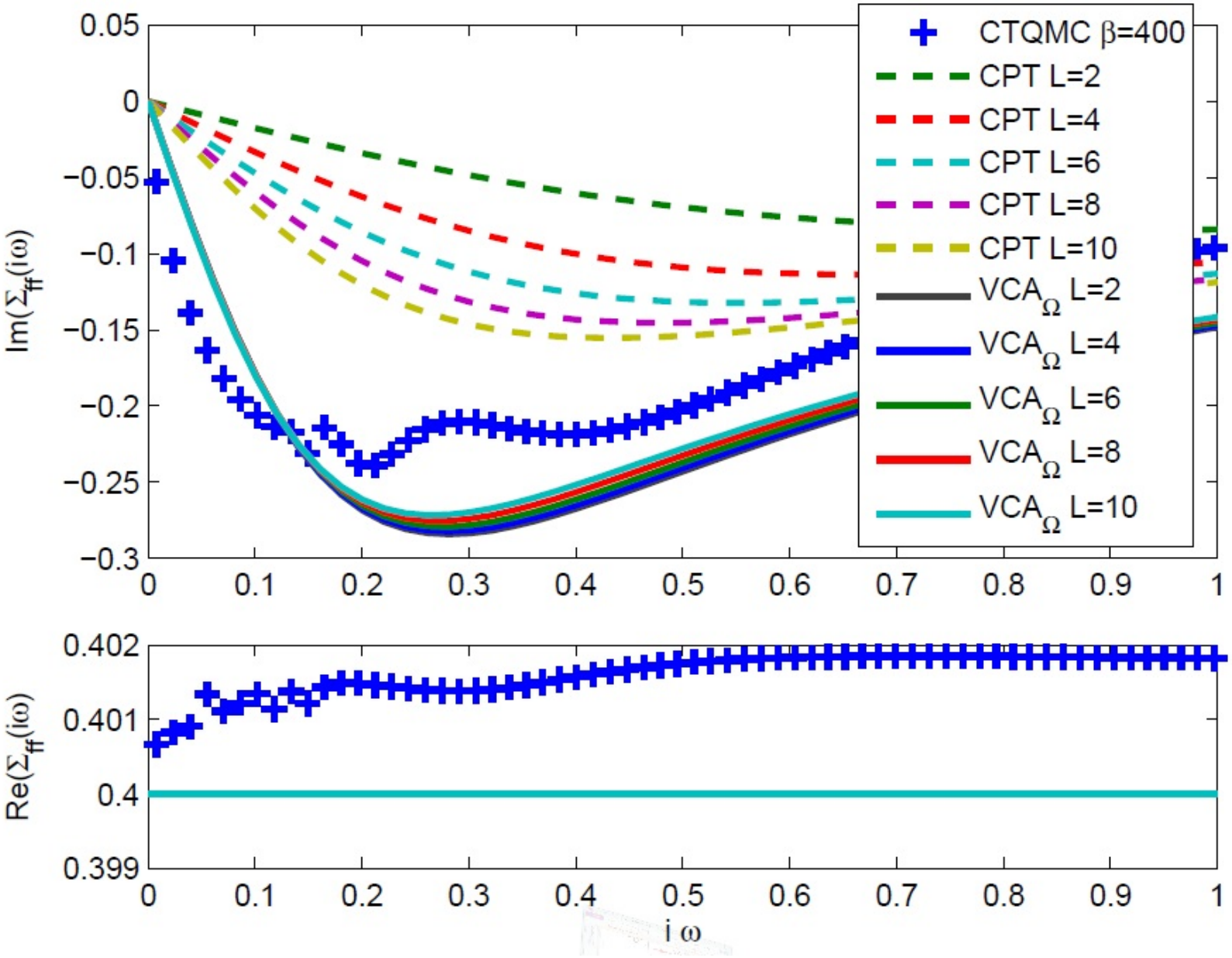


Static spin susceptibility

- The **static spin susceptibility** is **inversely proportional** to the Kondo temperature

$$\chi_m(U) = -\frac{d\left(\langle n_{f\uparrow}\rangle - \langle n_{f\downarrow}\rangle\right)}{d\,B}\bigg|_{B=0}.$$

Comparison to CTQMC



Nonequilibrium extension of VCA (I)

- Initial state: **three decoupled systems in equilibrium**

  left lead - cluster - right lead.

- At some time t_0 the **coupling is switched on**.
- We are interested in the long time **steady-state properties**.

Nonequilibrium extension of VCA (II)

- **Keldysh - formalism** to obtain steady-state properties.
- **VCA reformulated** in terms of self-consistently determined variational parameters where the self-consistency conditions are static expectation values (for example):

$$\left\langle \hat{n}^f_\sigma \right\rangle_{\text{cluster},\epsilon'_f,\epsilon'_s} \stackrel{!}{=} \left\langle \hat{n}^f_\sigma \right\rangle_{\text{CPT},\epsilon_f,\epsilon_s,\epsilon'_f,\epsilon'_s}$$

$$\sum_i^{L-1} \left\langle \hat{n}^i_\sigma \right\rangle_{\text{cluster},\epsilon'_f,\epsilon'_s} \stackrel{!}{=} \sum_i^{L-1} \left\langle \hat{n}^i_\sigma \right\rangle_{\text{CPT},\epsilon_f,\epsilon_s,\epsilon'_f,\epsilon'_s} .$$

- Green's functions calculated in **Keldysh space on the real energy axis**:

$$\tilde{\mathrm{G}}(\omega) = \begin{pmatrix} \mathrm{G}^{\mathrm{ret}}(\omega) & \mathrm{G}^{\mathrm{keld}}(\omega,\mu) \\ 0 & \mathrm{G}^{\mathrm{adv}}(\omega) \end{pmatrix}$$

- The initial $\mathrm{G}^{\mathrm{keld}}(\omega,\mu)$ of the decoupled system is given by

$$\mathrm{G}^{\mathrm{keld}}(\omega,\mu) = \left(\mathrm{G}^{\mathrm{ret}}(\omega) - \mathrm{G}^{\mathrm{adv}}(\omega)\right)\left(1 - 2\,p_{\mathrm{FD}}(\omega,\mu,\beta)\right)$$

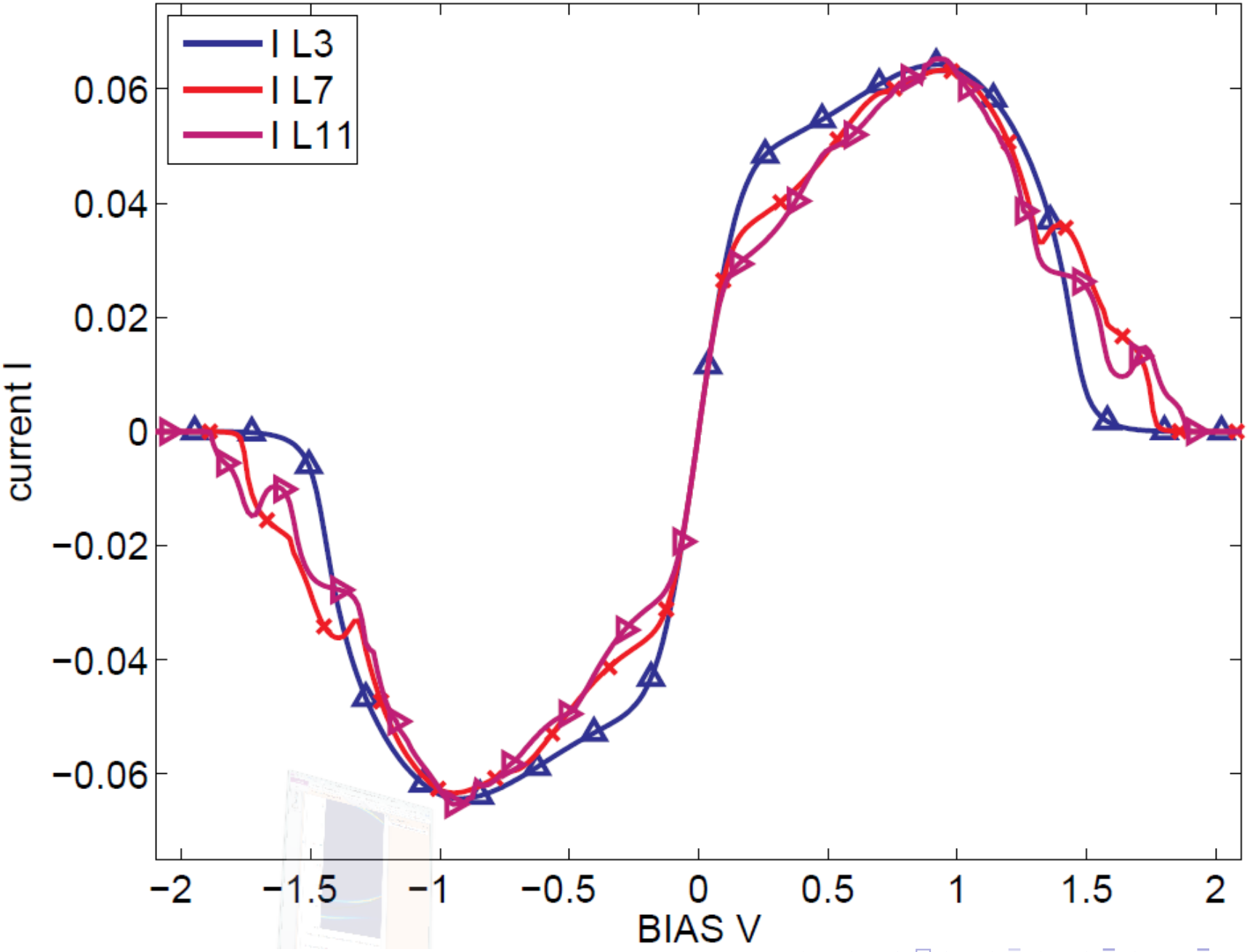
Current for a single impurity orbital

The expression for the current between sites i and j is given by:

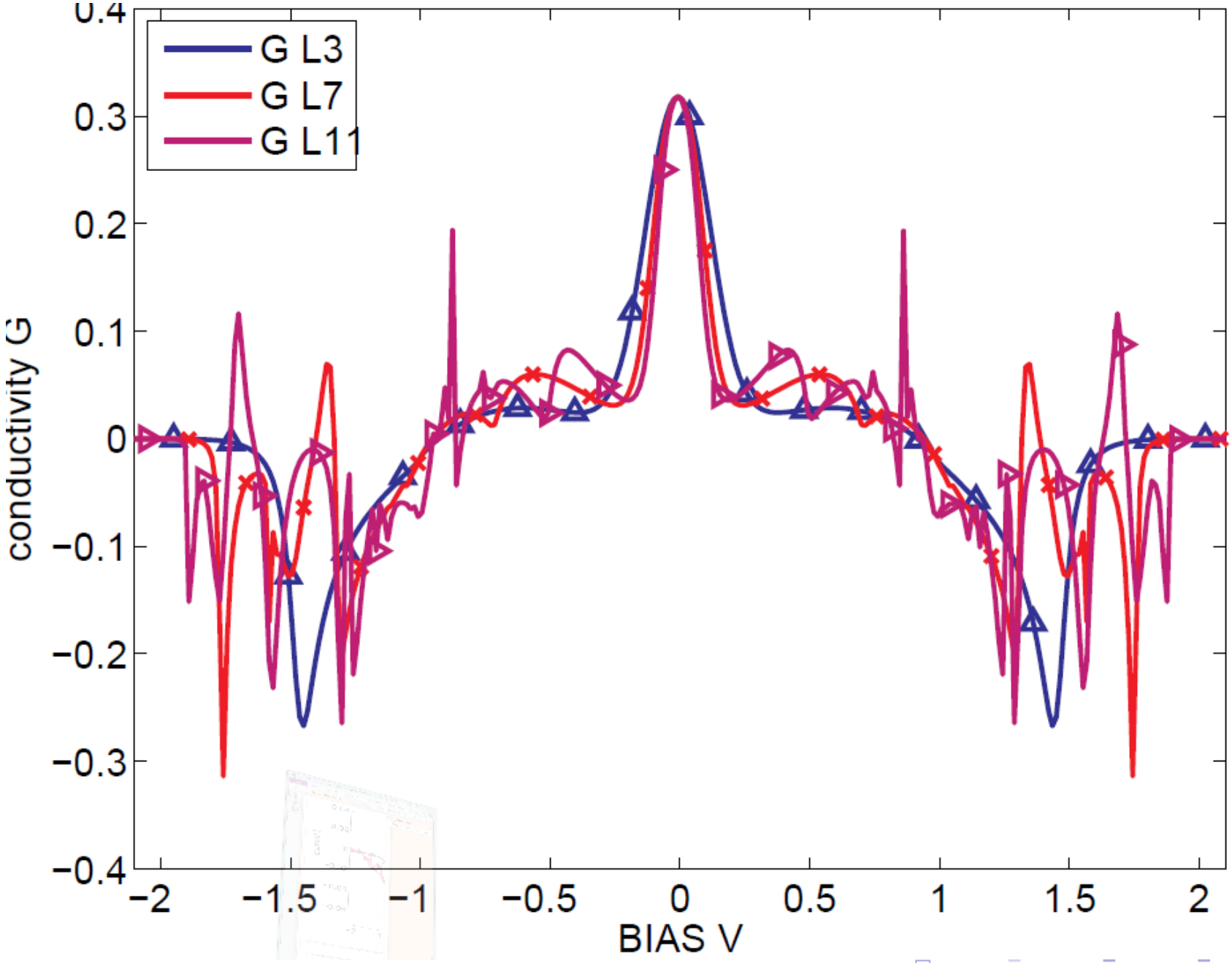
$$I_{ij} = t\,\mathrm{Re}\left(\mathrm{G}_{ij}^{\mathrm{keld}}(t=0)\right)$$
$$= \frac{t}{2}\int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}\mathrm{Re}\left(\mathrm{G}_{ij}^{\mathrm{keld}}(w) - \mathrm{G}_{ji}^{\mathrm{keld}}(w)\right)$$

The next slides show preliminary CPT results, showing spurious finite size effects. We expect these to be compensated by VCA.

Current for a single impurity orbital

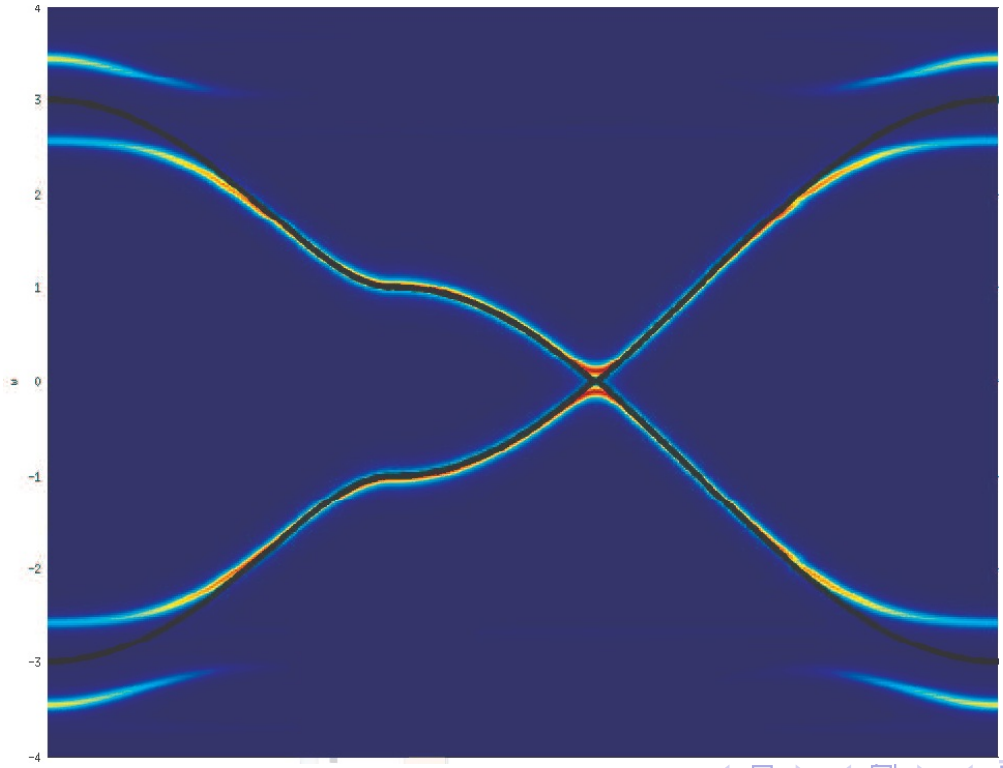


Conductance for a single impurity orbital



Future challenges

- **nonequilibrium** applications to (multilevel) quantum dots (under development)
- "magnetic" vacancies in **disordered** graphene (starting)



Thank You!

Thank you for your attention!