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

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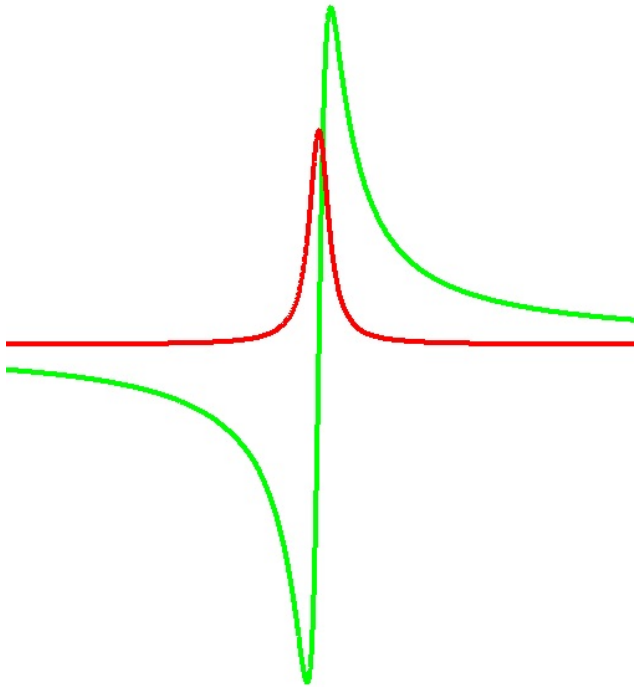
Generic lattice model

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

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

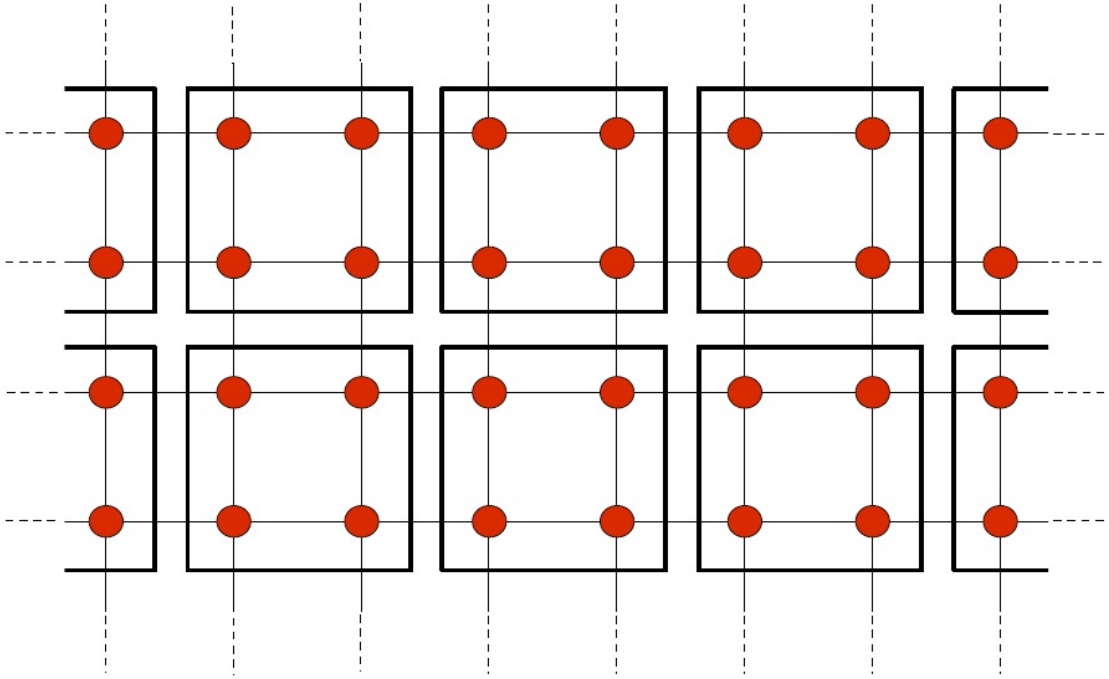
Atomic limit

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



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

Manybody Cluster Methods



Extrapolate cluster to thermodynamic limit:

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

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-Ladriére, 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

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

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

Cluster Perturbation Theory - Limits

CPT is exact for

- $t \to 0$,
- $U \to 0$,
- $L \to \infty$.

CPT captures **short-range correlations** exactly, long-range correlations are neglected.

Variational Cluster Approach[a]

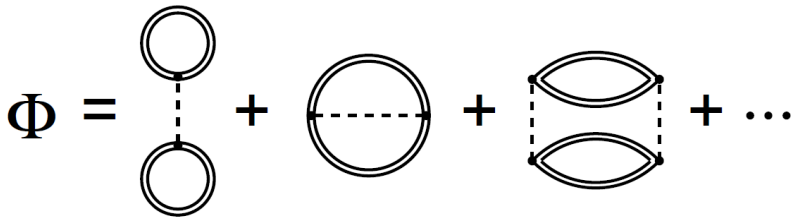
[a] M. Potthoff, M. Aichhorn, and C. Dahnken, Phys. Rev. Lett. 91, 206402 (2003)

- VCA = variational extension to CPT - rigorously developed within the **Self-Energy Functional Approach** (SFA)[ab],
- does **not** implement a variational principle in the sense of a Rayleigh-Ritz variational principle,
- is applicable to **broken-symmetry/ordered** phases.

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

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.

Legendre Transform of $\Phi[\mathsf{G}]$

It can be shown that

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

is **locally invertible**.
Legendre Transform of the Luttinger-Ward functional:

$$F[\Sigma] = \Phi[\Sigma] - \mathrm{Tr}\left\{\Sigma\mathsf{G}\right\}\,.$$

It can be shown that the generalized **grand potential functional** is given by:

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

Grand Potential Functional $\Omega[\Sigma]$

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

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

VCA Reference System (I)

Since systems which share the same interaction part $\hat{\mathcal{H}}_{II}(U)$ have the same $\Phi[\mathrm{G}]$ (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!)

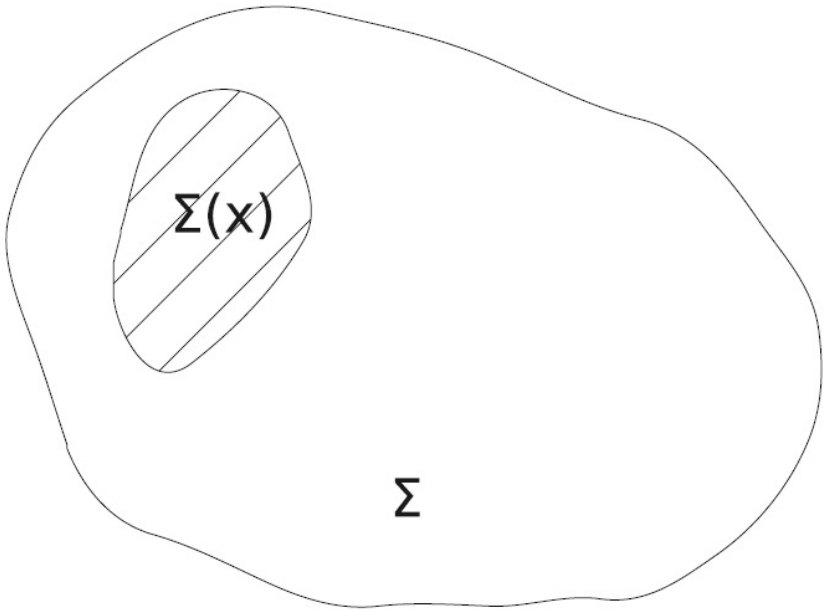
$$\Omega[\Sigma] = F[\Sigma] - \mathrm{Tr}\left\{\ln\left(-\mathsf{G}_0^{-1} + \Sigma\right)\right\}$$
$$\Omega'[\Sigma] = F[\Sigma] - \mathrm{Tr}\left\{\ln\left(-\mathsf{G}_0'^{-1} + \Sigma\right)\right\}$$

$$-\sum$$

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

Evaluation of the grand potential

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



VCA - Overview

- **Grand potential**

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

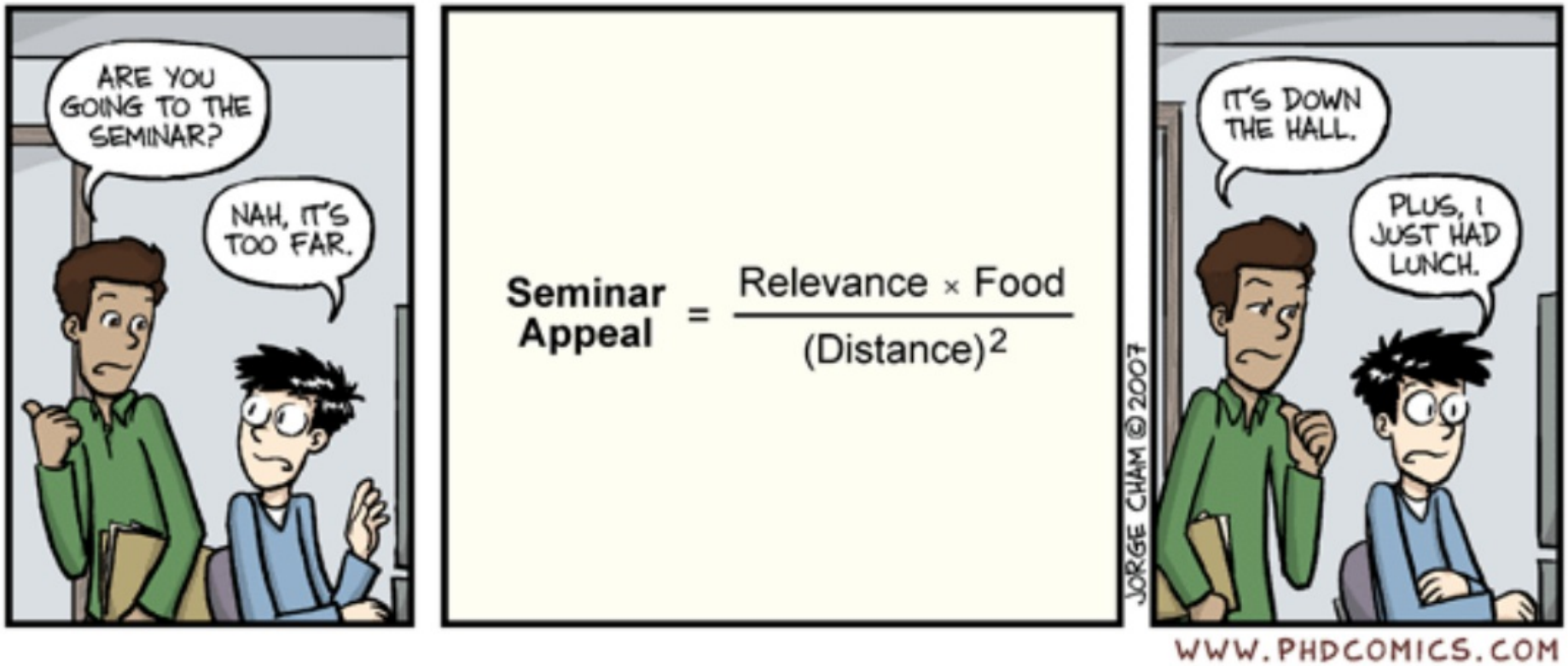
- **Stationarity condition:**

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

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

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

The matrix $\mathsf{T} = \mathsf{G}_0'^{-1} - \mathsf{G}_0^{-1}$ contains all single particle terms not included in the reference system (as in CPT) as well as the deviation, introduced by VCA, $\Delta\mathsf{x} \equiv \mathsf{x}' - \mathsf{x}$ of the single-particle parameters of the reference system x' with respect to the ones of the original system x.


ARE YOU GOING TO THE SEMINAR?
NAH, IT'S TOO FAR.
Seminar Appeal = Relevance × Food / (Distance)²
IT'S DOWN THE HALL.
PLUS, I JUST HAD LUNCH.
JORGE CHAM © 2007
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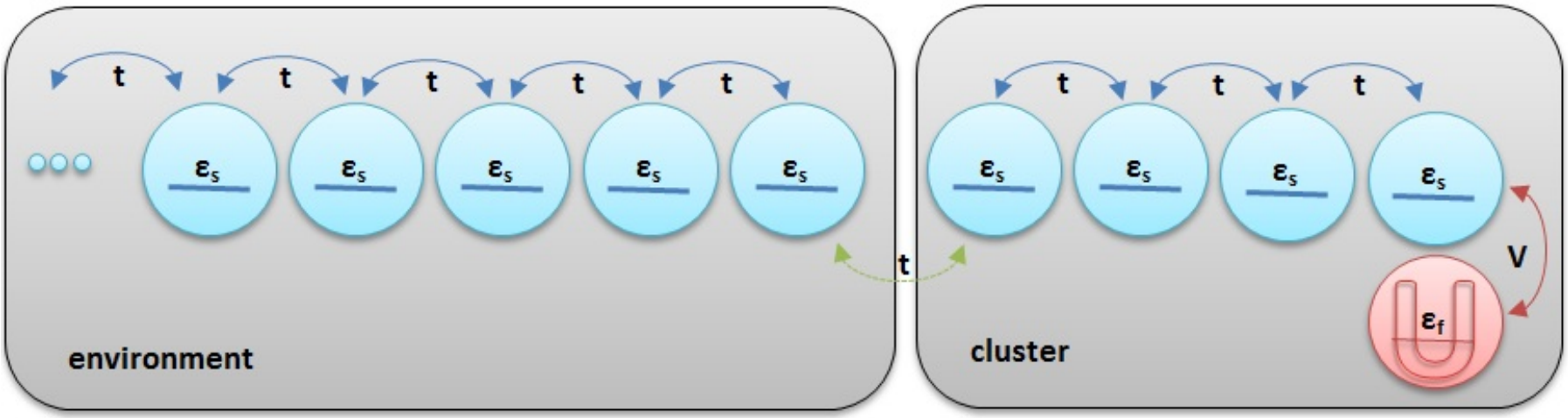
Single Impurity Anderson Model - Cluster decomposition



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):

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

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.

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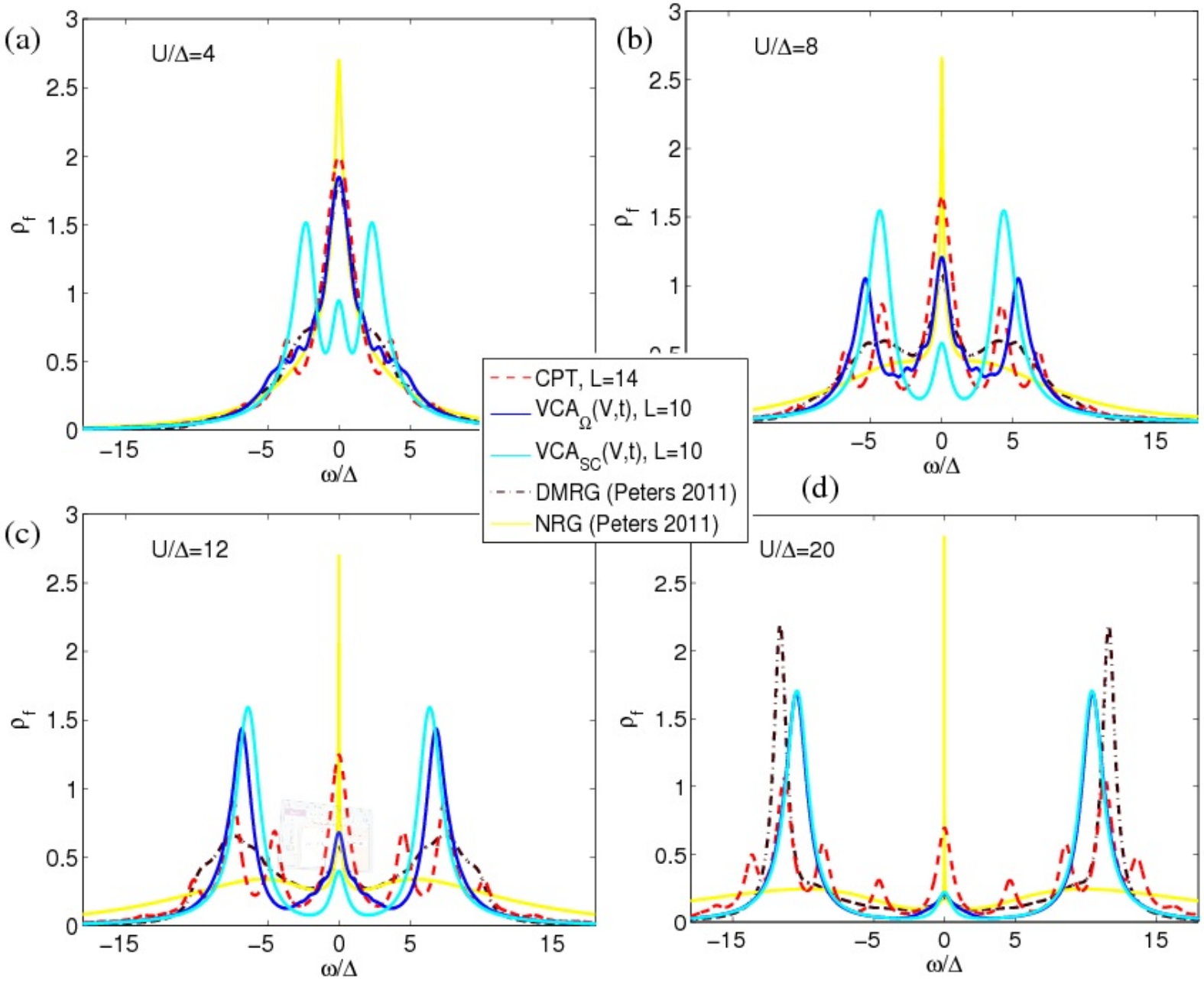
[a] C. Karrasch, R. Hedden, R. Peters, T. Pruschke, K. Schönhammer, and V. Meden, J. Phys.: Condensed Matter 20, 345205 (2008)

[b] R. Peters, 1103.5837 (2011)

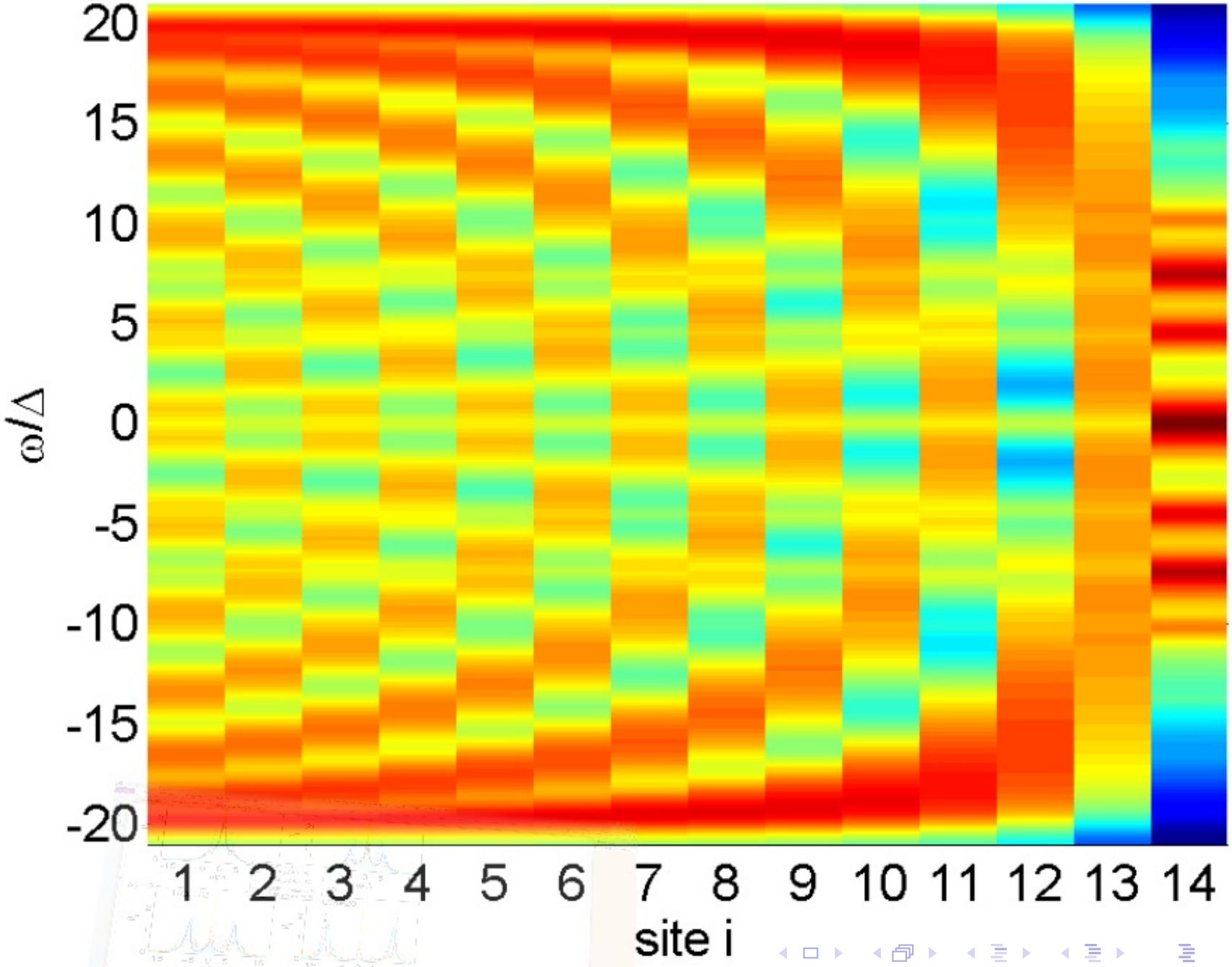
[c] T. Lobo, M. S. Figueira, and M. E. Foglio, Nanotechnology 21, 274007 (2010)

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

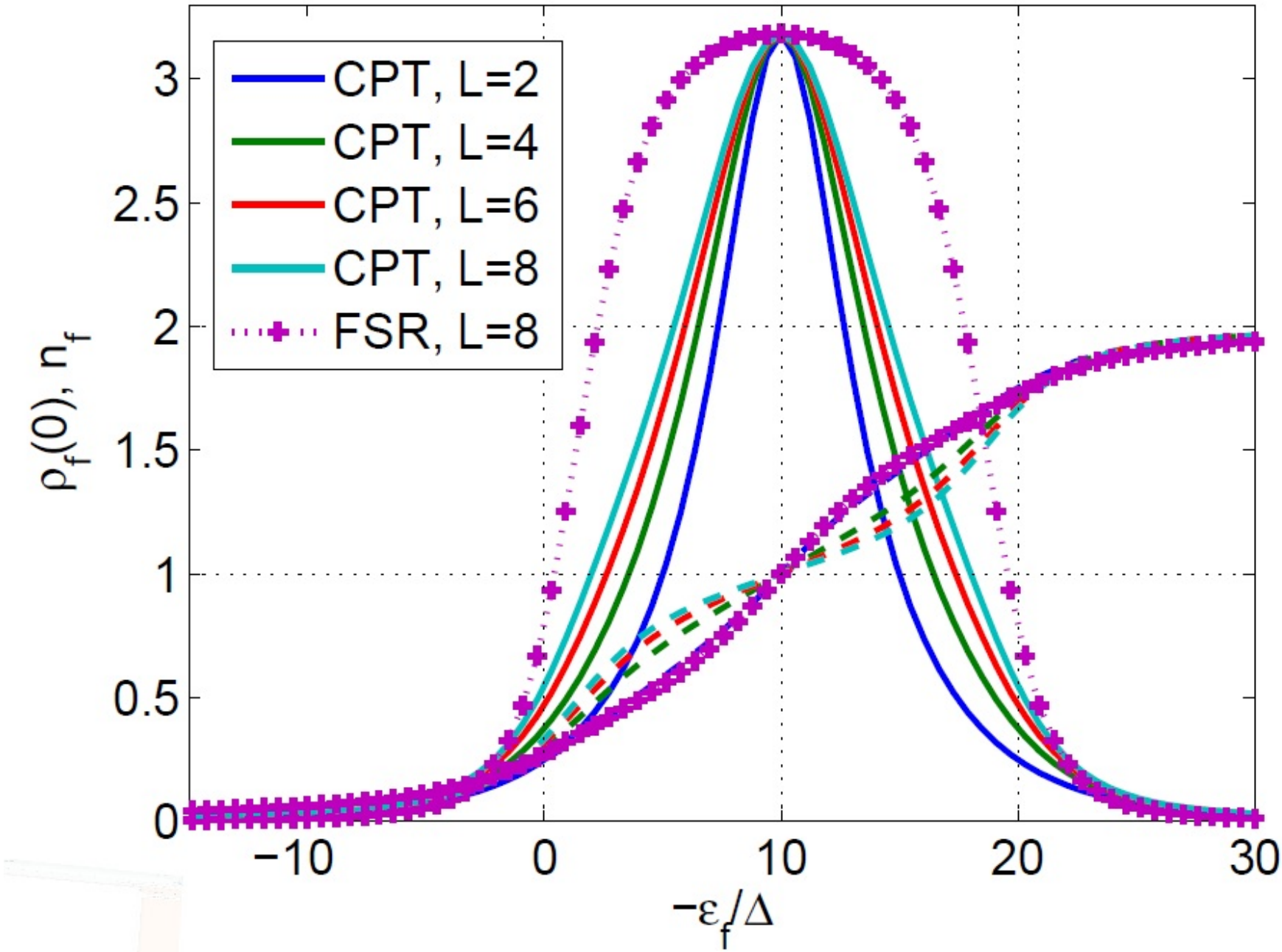
Spectral properties



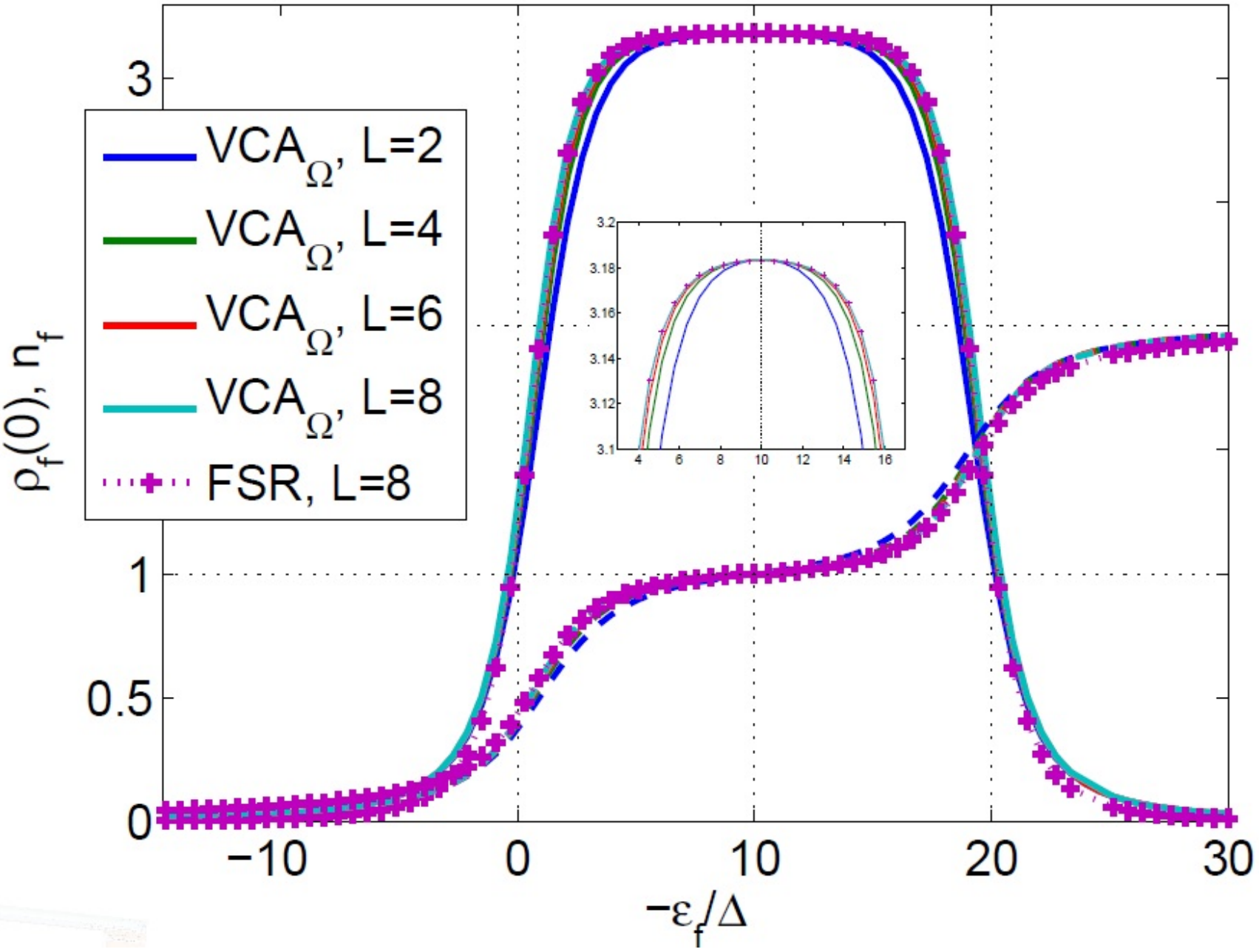
Spectral properties (spatial)



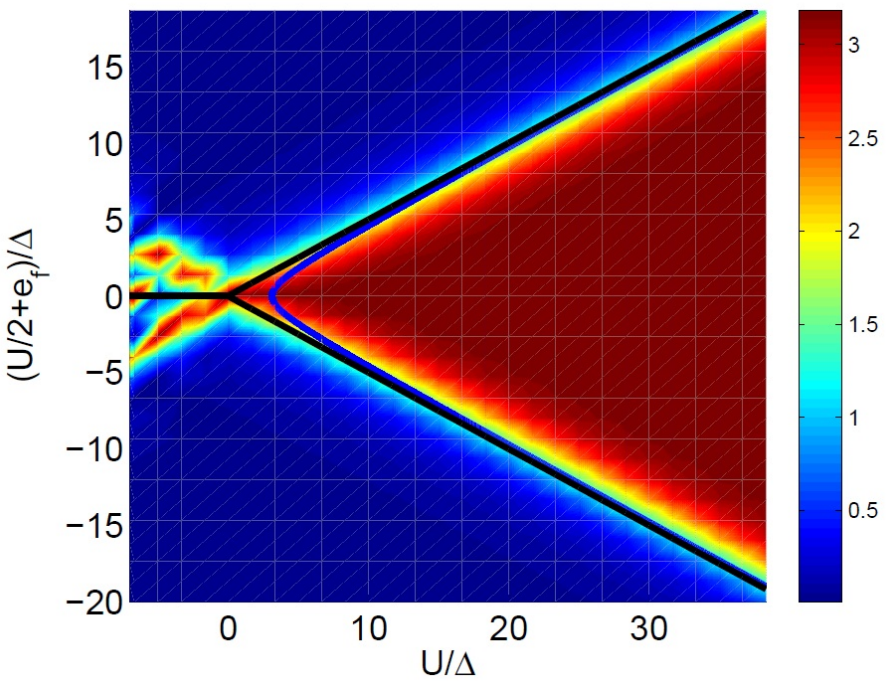
Impurity Occupation

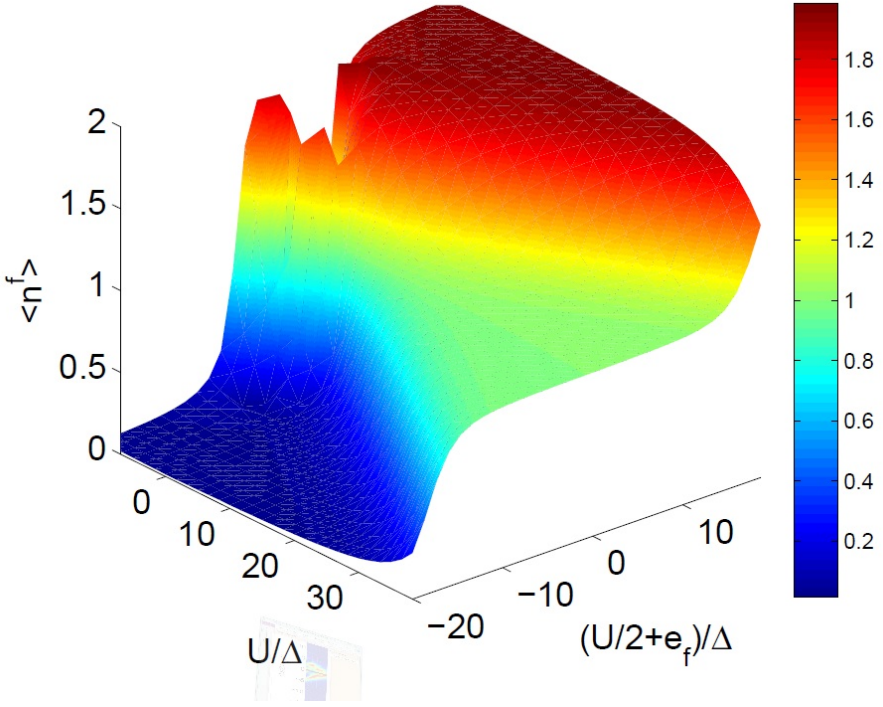


Impurity Occupation



"Crossover" diagram





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]

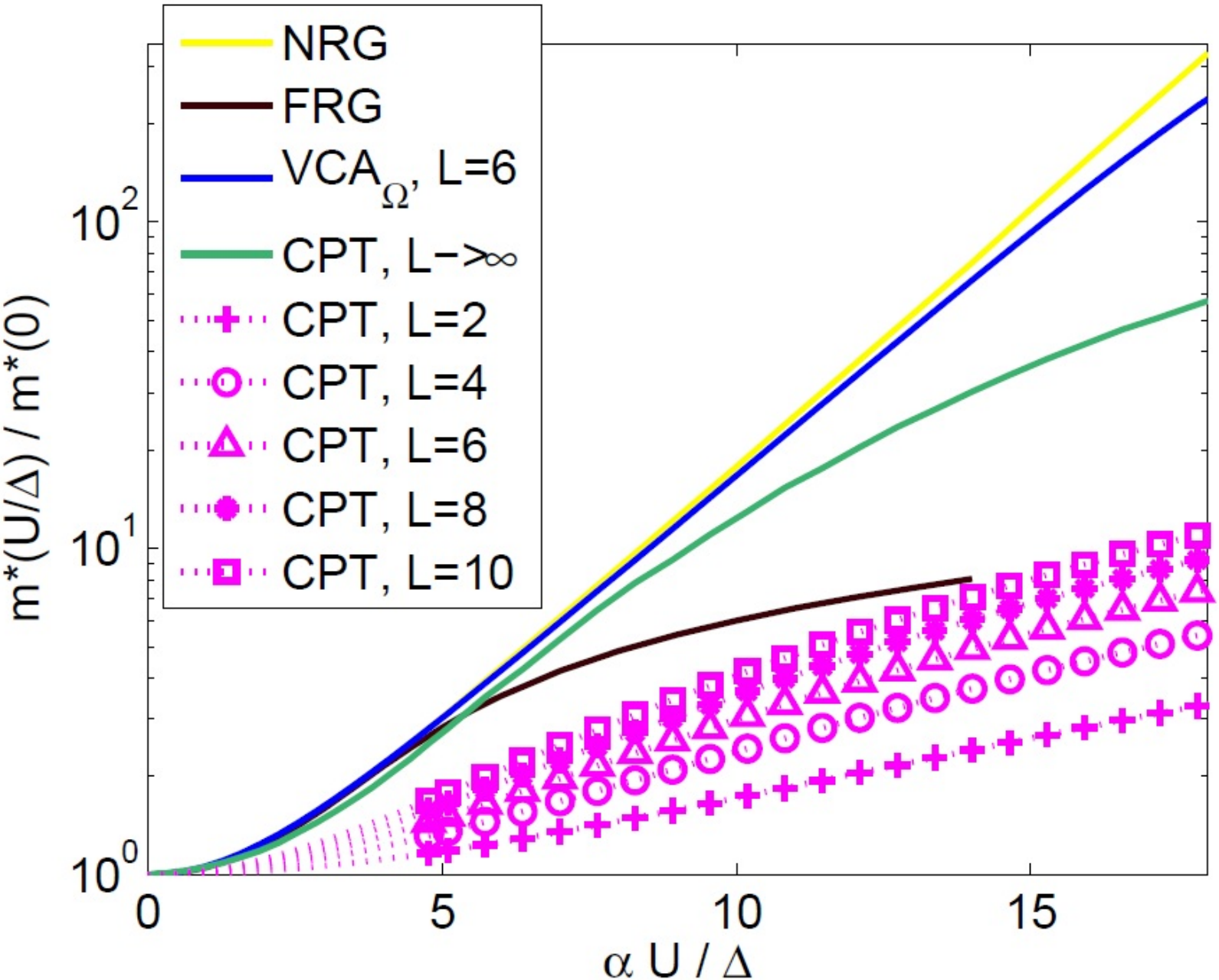
$$T_K = \sqrt{\frac{\Delta U}{2}}\, e^{-\gamma \frac{\pi}{8\Delta} U} \;, \quad \gamma = 1 \;.$$

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

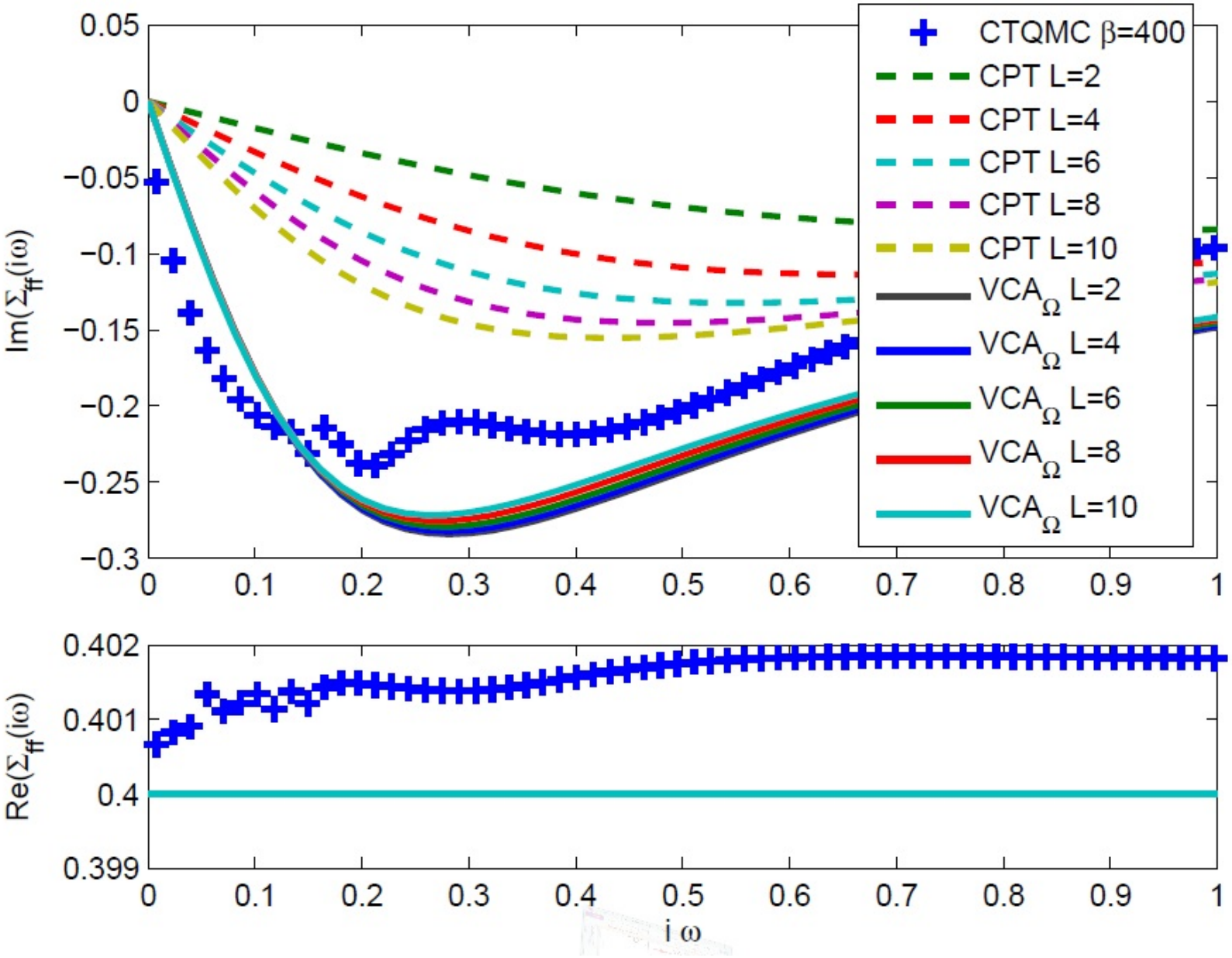
$$\gamma = 0.6511 \;.$$

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

Effective Mass



Comparison to CTQMC



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**

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):

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

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

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

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

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

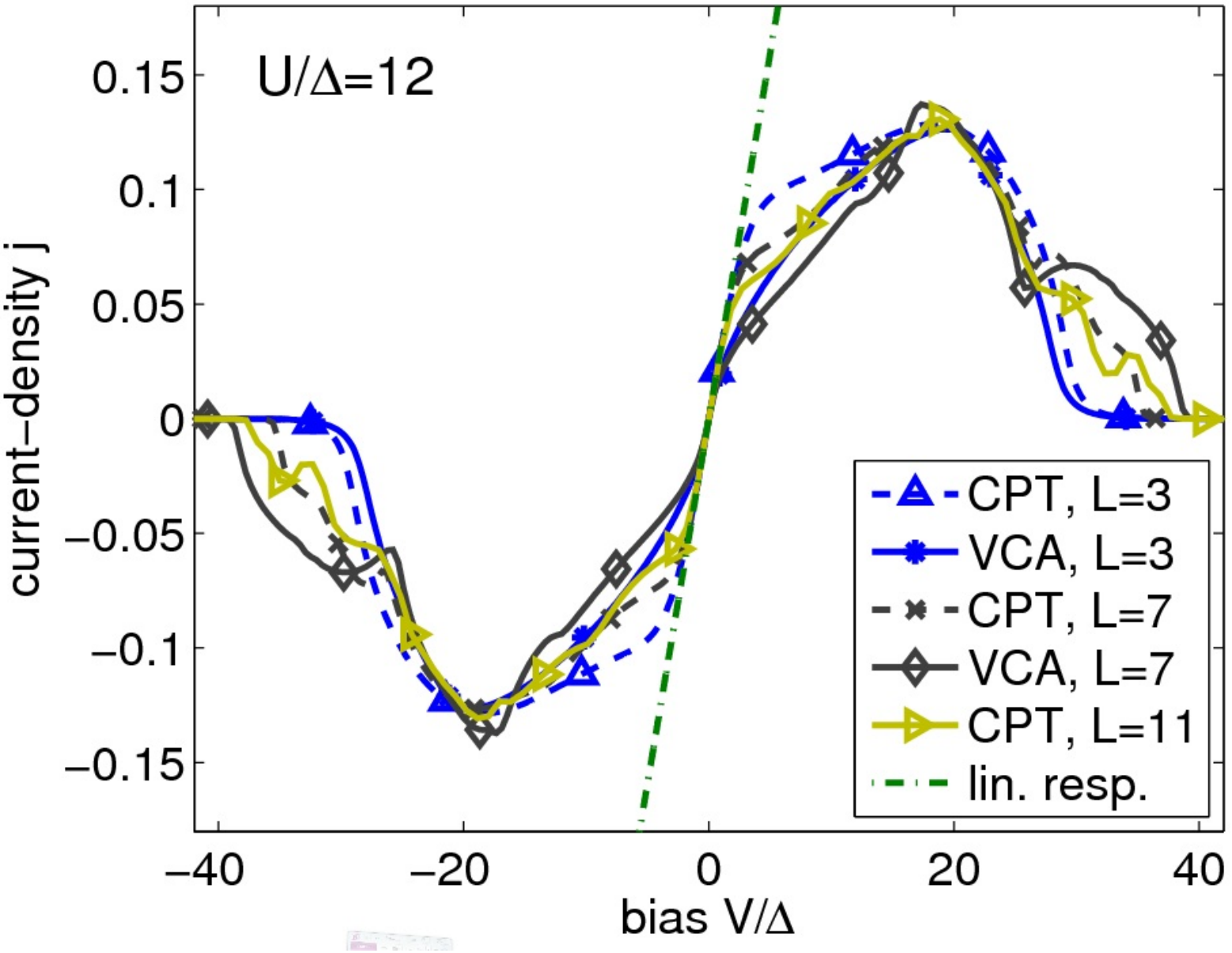
$$\mathsf{G}^{\text{keld}}(\omega,\mu) = \left(\mathsf{G}^{\text{ret}}(\omega) - \mathsf{G}^{\text{adv}}(\omega)\right)\,(1 - 2\,p_{\text{FD}}(\omega,\mu,\beta))$$

Current for a single impurity orbital

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

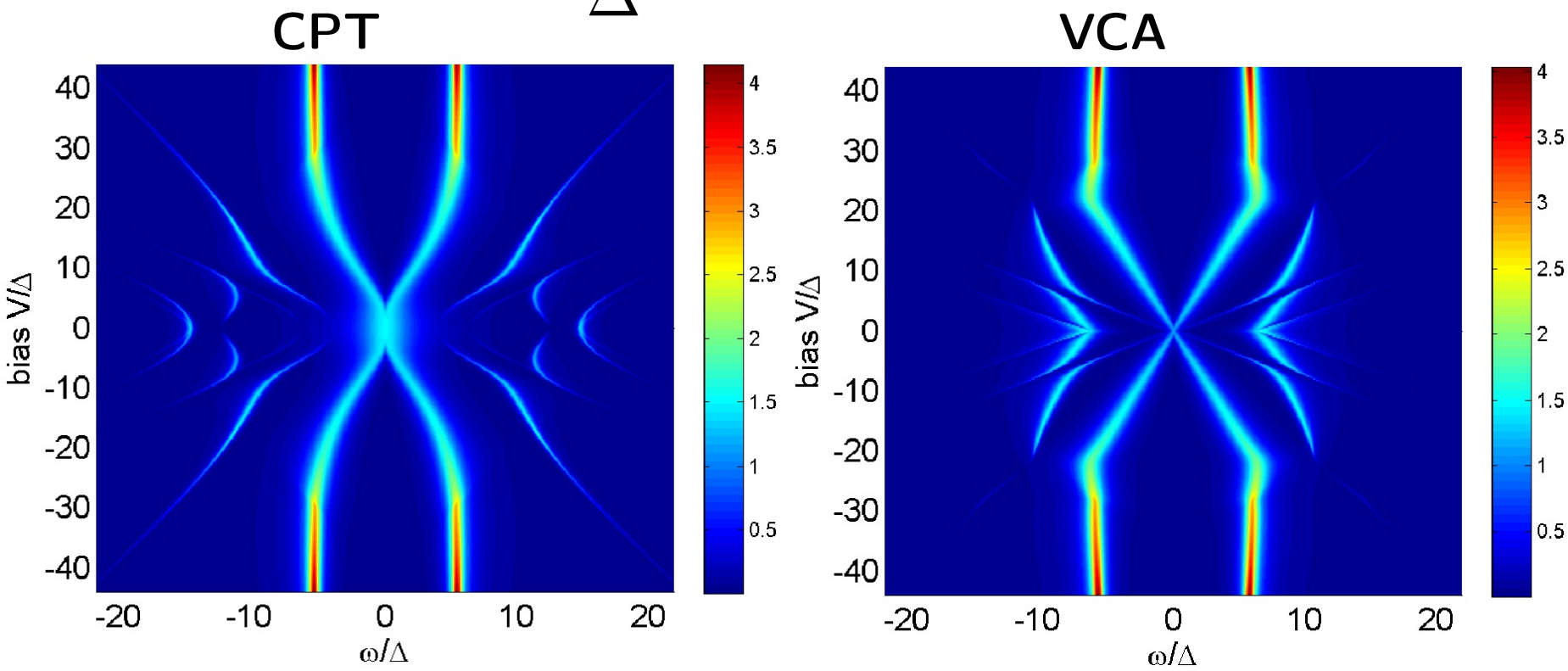
$$I_{ij} = t\,\mathrm{Re}\left(\mathsf{G}^{\mathsf{keld}}_{ij}(t=0)\right)$$
$$= \frac{t}{2}\int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}\mathrm{Re}\left(\mathsf{G}^{\mathsf{keld}}_{ij}(w) - \mathsf{G}^{\mathsf{keld}}_{ji}(w)\right)$$

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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