Evolution of Yu-Shiba-Rusinov (Andreev) bands in two-dimensional superconducting structures

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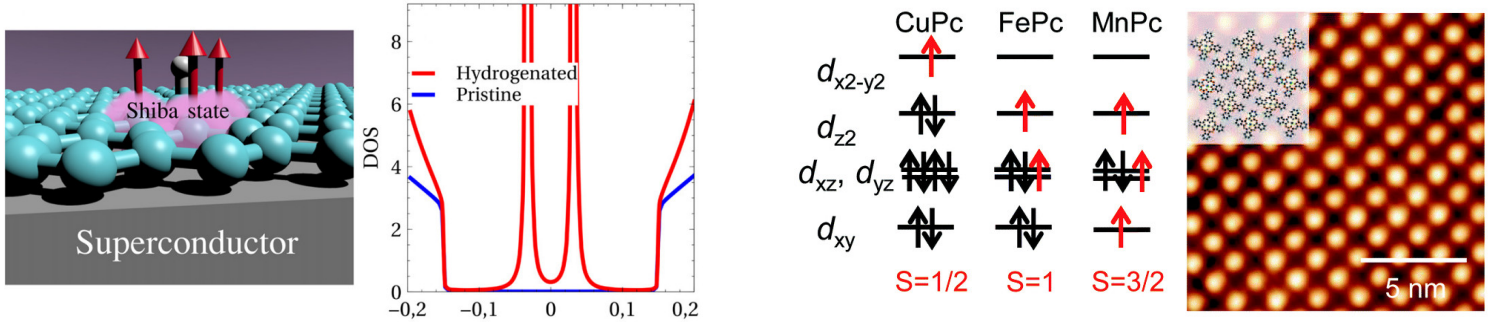
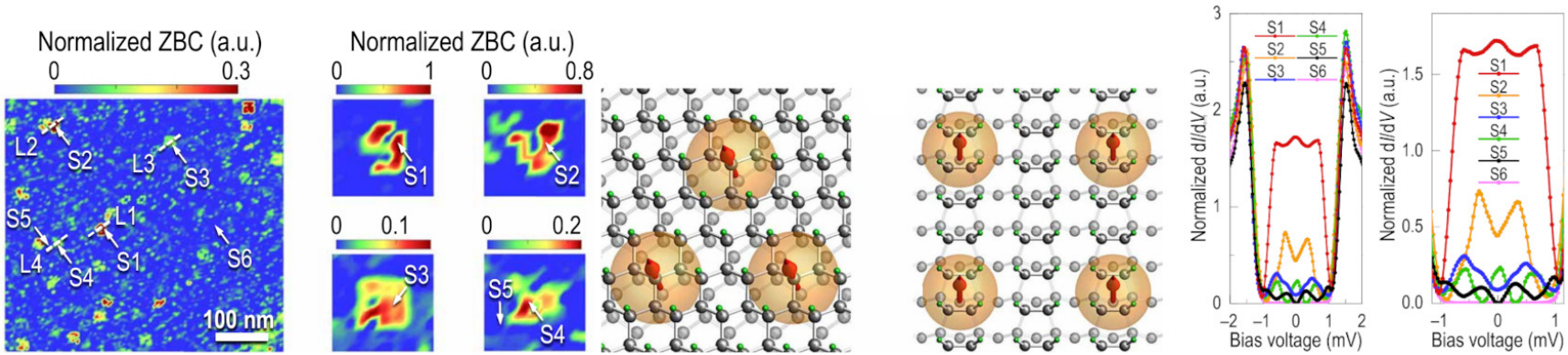
Motivation

lattice of impurities deposited on the surface of a conventional BCS superconductor - ideal playground for studying the interplay of antagonistic orders - magnetism and superconductivity

- hydrogenated superconducting graphene (1)
- transition metal (Mn, Fe, Cu) phtalocyanines on Pb or In (3,4)

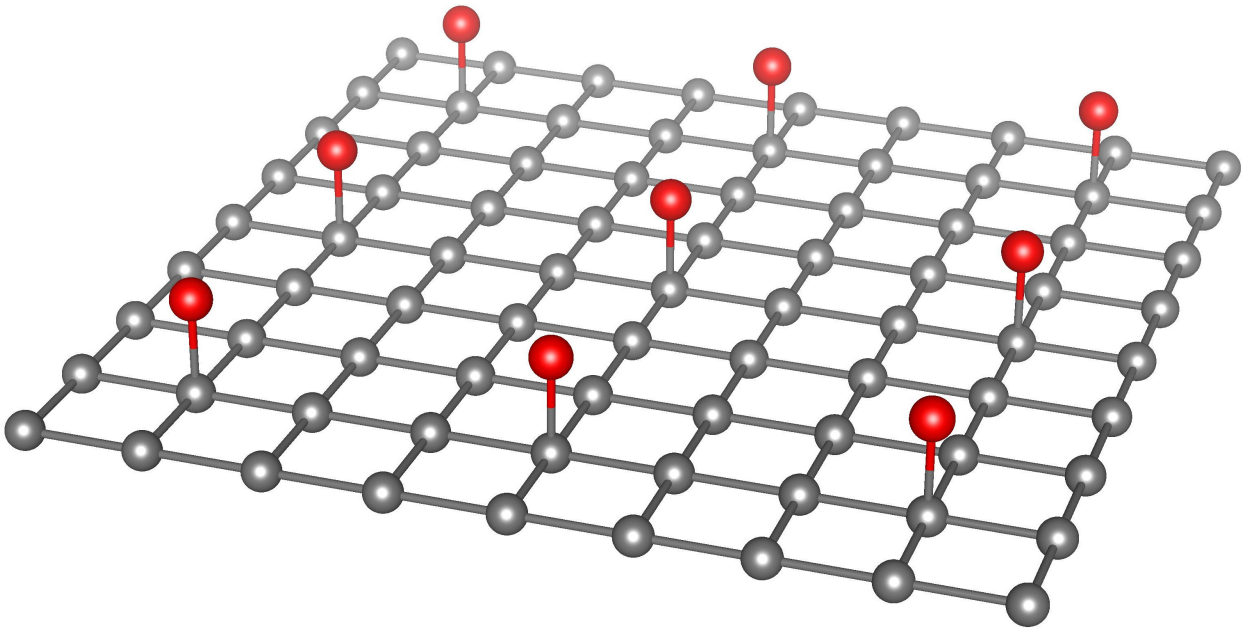


- boron-doped diamond coated with hydrogen layer (2)



(1) J. L. Lado and J. Fernández-Rossier, 2D Mater. **3**, 025001 (2016).
(2) G. Zhang *et al.*, Sci. Adv. **6**, aaz2536 (2020).
(3) S. Yoshizawa *et al.*, Nano Letters **17**, 2287 (2017).
(4) T. Uchihashi *et al.*, Mol. Syst. Des. Eng. **4**, 511 (2019).

lattice of impurities deposited on the surface of a conventional BCS superconductor



superconducting periodic Anderson model:

- **conduction band** with hopping and local attractive interaction (electron-phonon)
- **impurity band** with local repulsive interaction (Coulomb)
- impurities interact only via the hybridization with the conduction band, not directly (no hopping in the impurity band)

This model was already employed and solved using DMFT (1) and used to study reentrant behavior of superconductivity in f-electron superconductors (2).

(1) D. J. Luitz and F. F. Assaad, Phys. Rev. B **81**, 024509 (2010).
(2) W. V. van Gerven Oei and D. Tanasković J. Phys.: Condens. Matter **32** 325601 (2020).

- Hamiltonian

$$\mathcal{H} = \mathcal{H}_d + \mathcal{H}_c + \mathcal{H}_{\text{hyb}}$$

- conduction band: attractive interaction is treated on static mean field (BCS) level

$$\mathcal{H}_c = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}\sigma} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - \Delta \sum_{\mathbf{k}} (c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} + \text{H.c.}), \qquad \varepsilon_{\mathbf{k}\sigma} = \varepsilon_{\mathbf{k}} - \mu - \sigma H$$

- superconducting order parameter:

$$\Delta = g \sum_{\mathbf{k}} \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle \equiv g \sum_{\mathbf{k}} \langle c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} \rangle$$

- non-dispersive correlated band (impurities) - no kinetic term:

$$\mathcal{H}_d = \sum_{i\sigma} \varepsilon_{i\sigma} d^\dagger_{i\sigma} d_{i\sigma} + U \sum_i d^\dagger_{i\uparrow} d_{i\uparrow} d^\dagger_{i\downarrow} d_{i\downarrow}, \qquad \varepsilon_{i\sigma} = \varepsilon_i - \mu - \sigma H$$

- coupling:

$$\mathcal{H}_{\text{hyb}} = -\sum_{\mathbf{k}\sigma} (V_{\mathbf{k}\sigma} d^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \text{H.c.}), \qquad d^\dagger_{\mathbf{k}\sigma} = \frac{1}{\sqrt{N}} \sum_i e^{-i\mathbf{k}\cdot\mathbf{r}_i} d^\dagger_{i\sigma}$$

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- Nambu double-spinor $\psi_{\mathbf{k}}$ and the 4×4 matrix $E_{\mathbf{k}}$:

$$\psi_{\mathbf{k}} = \begin{pmatrix} d_{\mathbf{k}\uparrow} \\ d^{\dagger}_{-\mathbf{k}\downarrow} \\ c_{\mathbf{k}\uparrow} \\ c^{\dagger}_{-\mathbf{k}\downarrow} \end{pmatrix}, \quad E_{\mathbf{k}} = \begin{pmatrix} \varepsilon_{\uparrow} & 0 & -V_{\mathbf{k}\uparrow} & 0 \\ 0 & -\varepsilon_{\downarrow} & 0 & V_{-\mathbf{k}\downarrow} \\ -V_{\mathbf{k}\uparrow} & 0 & \varepsilon_{\mathbf{k}\uparrow} & -\Delta \\ 0 & V_{-\mathbf{k}\downarrow} & -\Delta & -\varepsilon_{-\mathbf{k}\downarrow} \end{pmatrix}$$

- Hamiltonian in Nambu formalism:

$$\mathcal{H} = \sum_{\mathbf{k}} \psi^{\dagger}_{\mathbf{k}} E_{\mathbf{k}} \psi_{\mathbf{k}} + U \sum_{i} d^{\dagger}_{i\uparrow} d_{i\uparrow} d^{\dagger}_{i\downarrow} d_{i\downarrow}$$

- Nambu Green function and the Dyson equation:

$$G_0(\mathbf{k}, \omega) = [\omega I - E_{\mathbf{k}}]^{-1}, \quad G(\mathbf{k}, \omega) = [G_0^{-1}(\mathbf{k}, i\omega) - \Sigma(\mathbf{k}, \omega)]^{-1}$$

- correlation-induced self-energy: only in the d-electron sector

$$\Sigma(\mathbf{k}, \omega) = \begin{pmatrix} \Sigma_d & \mathcal{S}_d & 0 & 0 \\ \bar{\mathcal{S}}_d & \bar{\Sigma}_d & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

c-electrons feel correlations only via hybridization V

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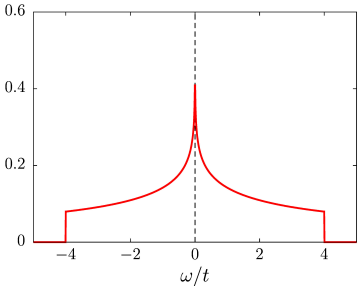
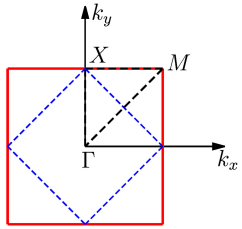
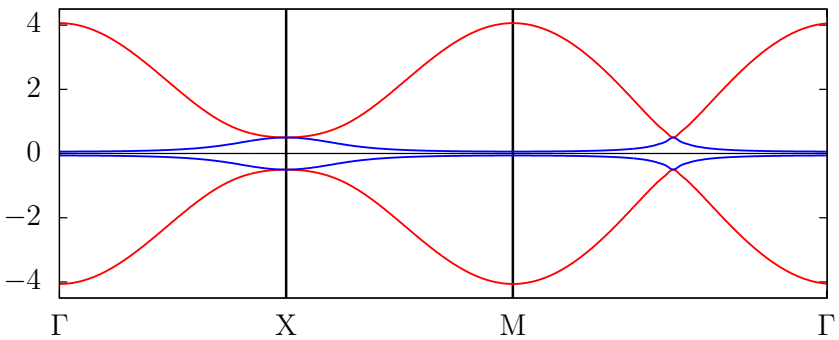
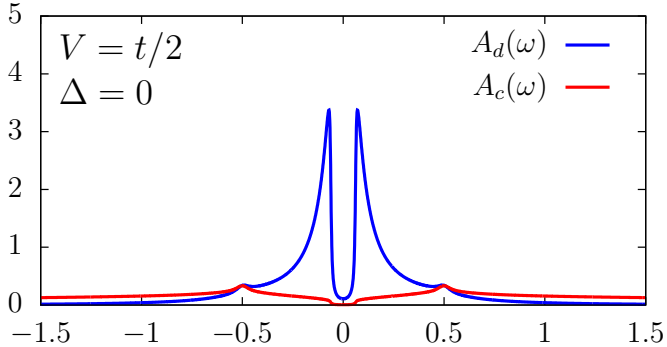
- square lattice: $\varepsilon_{\mathbf{k}} = -2t[\cos(ak_x) + \cos(ak_y)]$

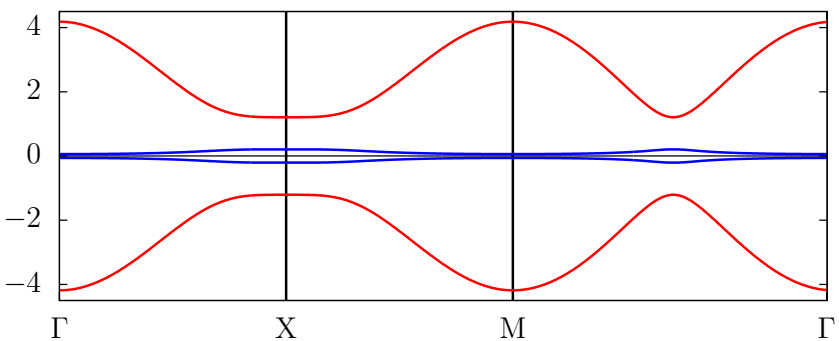


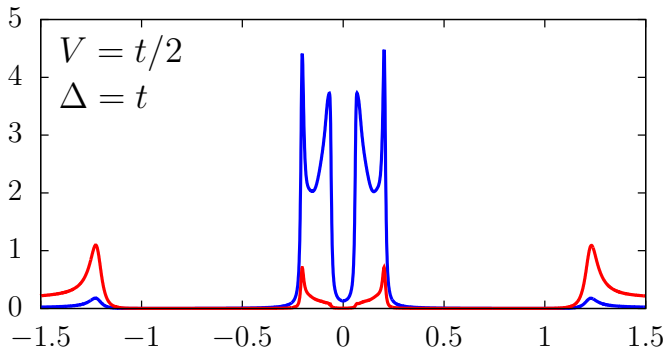


- band structure: zeros of Det $G_0^{-1}(\mathbf{k}, \omega)$ and local density of states for $V = t/2$:









- what about U?

- DMFT maps the lattice model on the local impurity model: on our case the superconducting impurity Anderson model (SCIAM) with self-consistently determined bath (hybridization function)
- it neglects all spatial correlations, self-energy becomes local: $\Sigma(\mathbf{k},\omega) \approx \Sigma(\omega)$
- local element of the Green function:

$$G_{\mathrm{loc}}(\omega) = \sum_{\mathbf{k}} G(\mathrm{k},\omega) = \begin{pmatrix} G_{d,\mathrm{loc}} & G_{dc,\mathrm{loc}} \\ G^{\dagger}_{dc,\mathrm{loc}} & G_{c,\mathrm{loc}} \end{pmatrix}$$

- d-electron bath Green function: input to the auxiliary impurity problem

$$\mathcal{G}(\omega) = [G^{-1}_{d,\mathrm{loc}}(\omega) + \Sigma(\omega)]^{-1}$$

- **solve the impurity model using your favourite solver for SCIAM:**
  result: $G_{\mathrm{imp}}(\omega)$ and $\Sigma_{\mathrm{imp}}(\omega) = \mathcal{G}^{-1}(\omega) - G^{-1}_{\mathrm{imp}}(\omega)$
- identify $\Sigma_d(\omega)$ with $\Sigma_{\mathrm{imp}}(\omega)$
- Dyson equation:

$$G(\mathbf{k},\omega) = [G_0^{-1}(\mathbf{k},\omega) - \Sigma(\omega)]^{-1}, \quad \Sigma(\omega) = \begin{pmatrix} \Sigma_d(\omega) & 0 \\ 0 & 0 \end{pmatrix}$$

- iterate until $G_{d,\mathrm{loc}}(\omega) = G_{\mathrm{imp}}(\omega)$
- hard part: solve the SCIAM

(1) A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996).

(2) G. Kotliar, S. Y. Savrasov, K. Haule, V. S. Oudovenko, O. Parcollet, and C. A. Marianetti, Rev. Mod. Phys. **78**, 865 (2006).

- continuous-time hybridization expansion quantum Monte Carlo (1)
- diagrammatic expansion in $\mathcal{H}_{\text{hyb}}$ around the 'atomic limit' $\mathcal{H}_d + \mathcal{H}_c$
- problem: Hamiltonian is not conserving
  solution: particle-hole transformation in the $\sigma = \downarrow$ segment (2):

$$d^\dagger_\uparrow \to d^\dagger_\uparrow, \quad c^\dagger_{\mathbf{k}\uparrow} \to c^\dagger_{\mathbf{k}\uparrow}, \quad d^\dagger_\downarrow \to d_\downarrow, \quad c^\dagger_{\mathbf{k}\downarrow} \to c_{-\mathbf{k}\downarrow}$$

- it maps the SC model on non-SC: $\langle c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} \rangle \to \langle c^\dagger_{\mathbf{k}\uparrow} c_{\mathbf{k}\downarrow} \rangle$,
  with attractive interaction $-U$,
  local energy ε becomes the magnetic field $-H$ and vice versa.
- we use the TRIQS/CTHYB (triqs.github.io) implementation of the algorithm (3,4)

Pros and cons:

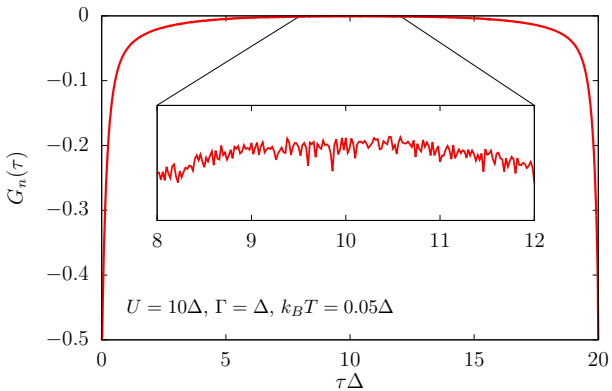
- ✔ CT-HYB provides 'numerically exact' solution to SCIAM: occupation numbers, c-band gap $\Delta = g \sum_{\mathbf{k}} \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle$, d-band induced pairing $\nu_d = \langle d_\downarrow d_\uparrow \rangle$, impurity density matrix...
- ✔ no fermionic sign problem
- ✘ works only in finite temperatures, comp. time scales as $t_c \sim T^{-2}$
- ✘ simulation is performed in imaginary time domain: no direct access to spectral functions w/o ill-defined analytic continuation $i\omega_n \to \omega + i0$

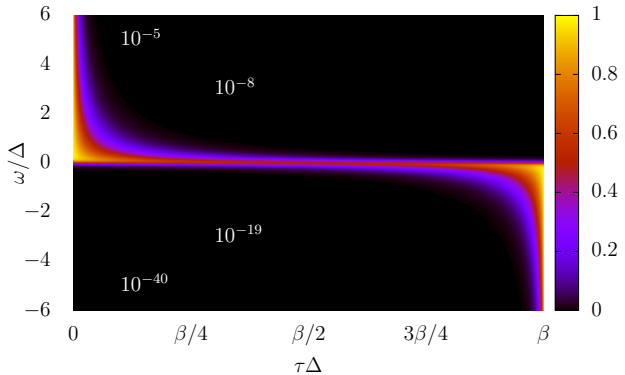
(1) E. Gull, A. J. Millis, A. I. Lichtenstein, A. N. Rubtsov, M. Troyer, and P. Werner, Rev. Mod. Phys. **83**, 349 (2011).
(2) D. J. Luitz and F. F. Assaad, Phys. Rev. B **81** 024509, (2010).
(3) O. Parcollet, M. Ferrero, T. Ayral, H. Hafermann, I. Krivenko, L. Messio, and P. Seth, Comput. Phys. Commun. **196**, 398 (2015).
(4) P. Seth, I. Krivenko, M. Ferrero, and O. Parcollet, Comput. Phys. Commun. **200**, 74 (2016).

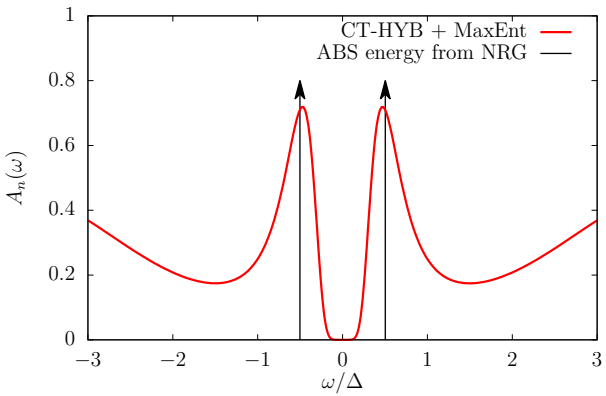
- CT-HYB Green function is calculated in imaginary time, no direct access to spectral functions
- analytic continuation $i\tau \rightarrow \omega$ of noisy data is an ill-defined problem (there is an infinite number of spectral functions $A(\omega)$ which correspond to the same noisy $G(\tau)$
- $G(\tau)$ is surprisingly insensitive to small changes in $A(\omega)$
- inverse problem: solve an integral equation for $A(\omega)$ (direct problem $A(\omega) \rightarrow G(\tau)$ is easy)

$$G(\tau) = \int d\omega \frac{e^{-\tau\omega}}{1 + e^{-\beta\omega}} A(\omega)$$

- usual approach: Bayesian inference, e.g., maximum entropy method (1)
  example: Andreev states of superconducting impurity model:







- not reliable for spectra with sharp features, e.g, Andreev states/bands
- there are tricks how to increase the resolution

(1) M. Jarrell and J. E. Gubernatis, Phys. Rep. **269**, 133 (1996).

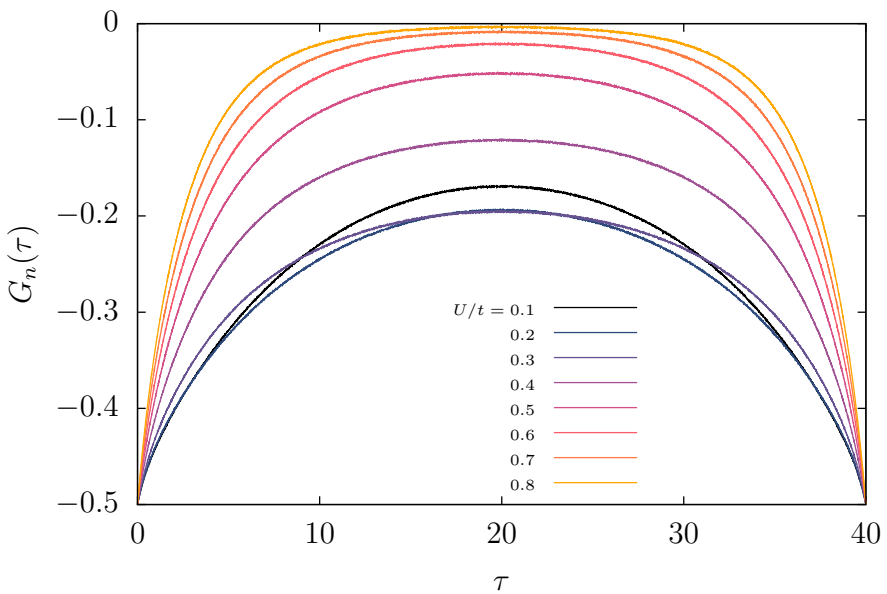
- Green function in imaginary time holds certain information about the value of the spectral function at the Fermi energy (1). Since

$$G(\tau) = \int d\omega \frac{e^{-\tau\omega}}{1+e^{-\beta\omega}} A(\omega), \qquad \beta = 1/k_B T$$

for $\tau = \beta/2$ (center of the imaginary time interval) we get

$$G(\beta/2) = \int d\omega \frac{A(\omega)}{2\cosh(\beta\omega/2)}$$

- $G(\beta/2)$ is a measure of the integrated spectral weight on an interval of few $k_B T$ around the Fermi energy.
- As $(\beta/2)\cosh^{-1}(\beta\omega/2) \to \pi\delta(\omega)$ for $\beta \to \infty$: $\beta G(\beta/2) \approx \pi A(0)$ for very low temperatures

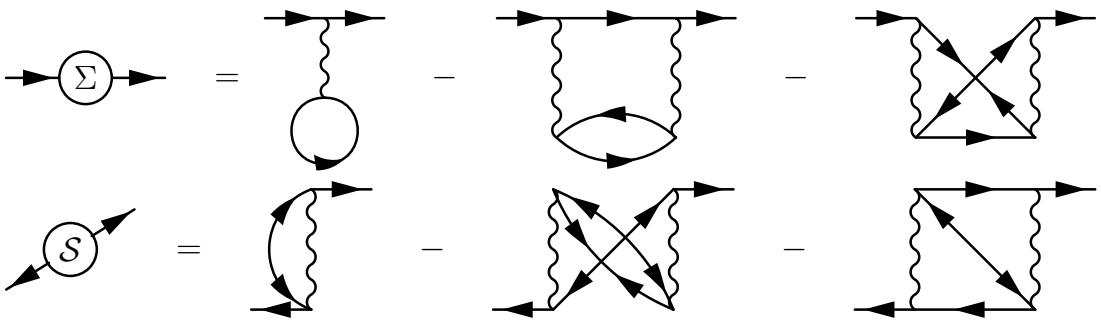


(1) A. Liebsch, Phys. Rev. Lett. **91**, 226401 (2003).

- simple approximate solver: second-order perturbation theory around the $U = 0$ limit (1)
- self-energy in imaginary time: Hartree-Fock and dynamic correction up to U^2:

$$\Sigma_\sigma(\tau) = U\mathcal{G}_{-\sigma}(0^-) - U^2\bar{\mathcal{G}}_{-\sigma}(-\tau)[\mathcal{G}_\uparrow(\tau)\bar{\mathcal{G}}_\downarrow(\tau) - \mathcal{F}_\uparrow(\tau)\bar{\mathcal{F}}_\downarrow(\tau)]$$

$$\mathcal{S}_\sigma(\tau) = U\mathcal{F}_{-\sigma}(0^-) - U^2\mathcal{F}_{-\sigma}(-\tau)[\mathcal{G}_\uparrow(\tau)\bar{\mathcal{G}}_\downarrow(\tau) - \mathcal{F}_\uparrow(\tau)\bar{\mathcal{F}}_\downarrow(\tau)]$$

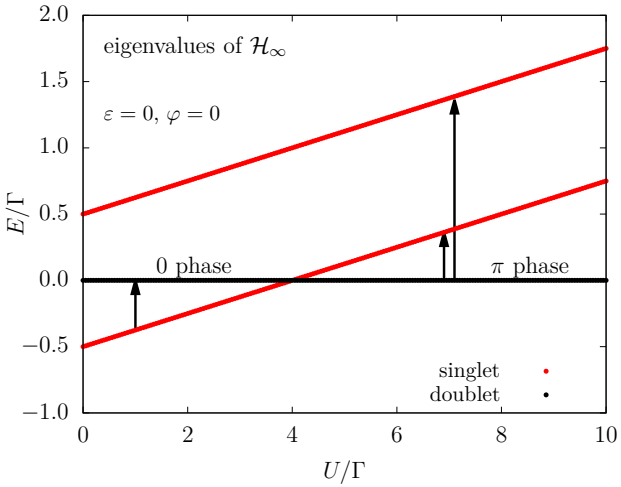


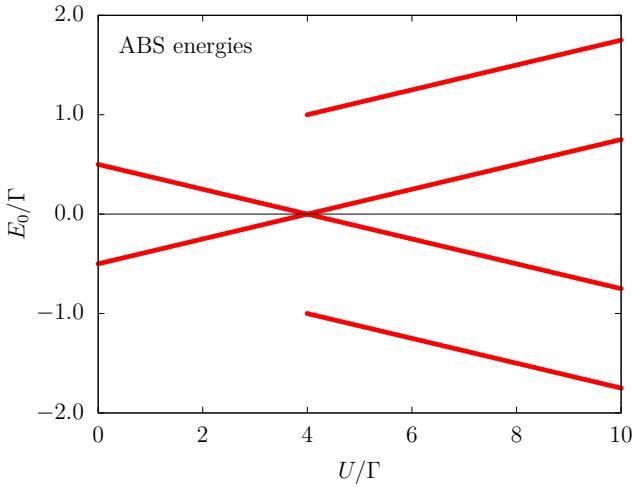
Pros and cons:

- ✔ IPT can be implemented directly in real-frequency domain or we can use the Pade analytic continuation from imaginary time
- ✘ only approximate solution, works best around half-filling
- ✘ cannot describe the strongly correlated (Kondo) regime
- ✘ IPT can fail in the case of a spinful ground state of the impurity model (3)

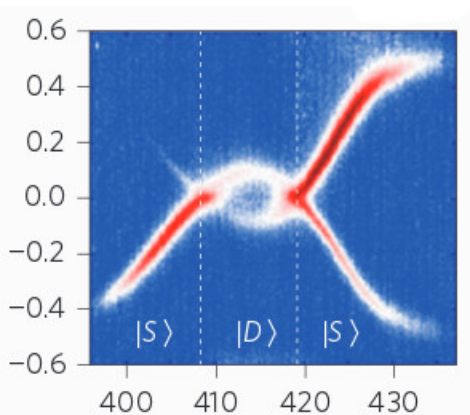
(1) H. Kajueter and G. Kotliar, Phys. Rev. Lett. **77**, 131 (1996).
(2) A. Garg, H. R. Krishnamurthy, and M. Randeria, Phys. Rev. B **72**, 024517 (2005).
(3) M. Žonda, V. Pokorný, V. Janiš, and T. Novotný, Sci. Rep. **5**, 8821 (2015).

- low-energy spectrum of SCIAM consists of two spin-singlets and one spin-doublet
- a quantum phase transition separates phases with singlet (0) and doublet (π) ground state





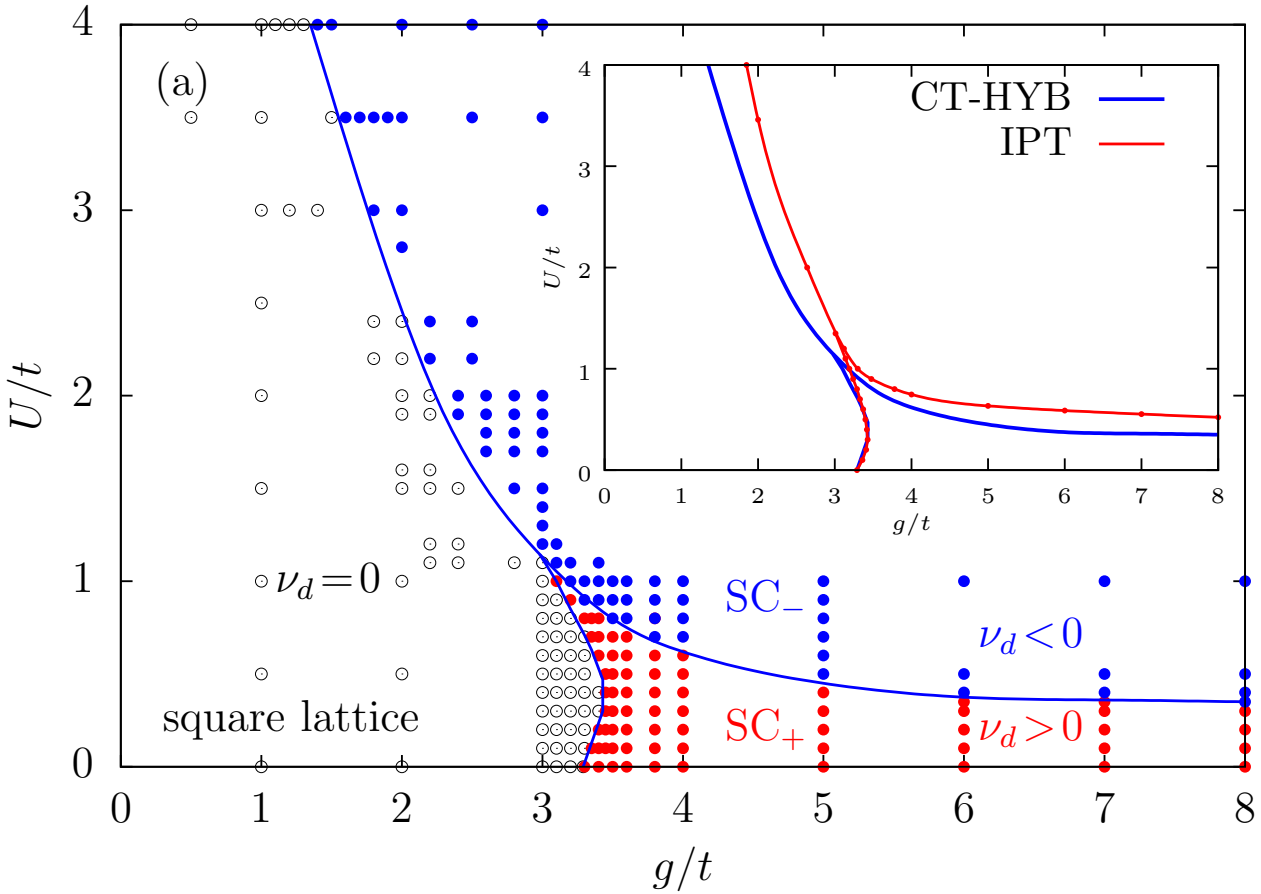
- QPT is characterized by
  - the crossing of the in-gap YSR states ar the Fermi energy
  - change of sign of the induced pairing on the impurity
  - change of the direction of the DC Josephson current



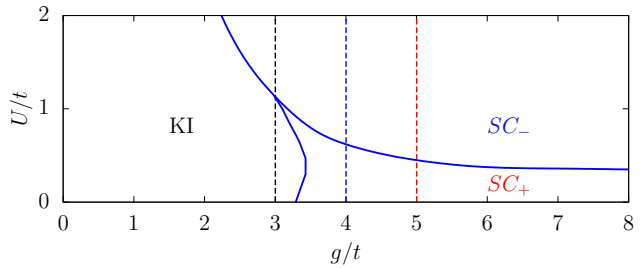
E. J. H. Lee et al., Nat. Nano. **9**, 79 (2014).

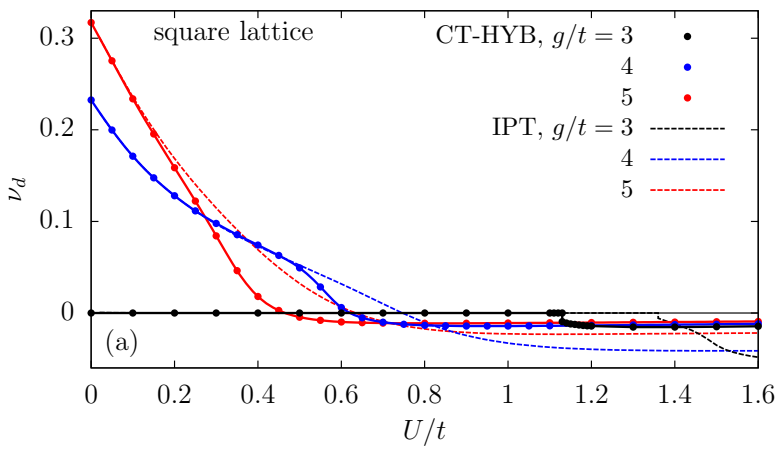
- impurity quantum phase transition: happens on a zero-dimensional subsystem (local impurity) connected to an infinite system (lead)
- as the $U = 0$ case is always a singlet, diagrammatic perturbation techniques in U cannot describe the doublet phase: no way to switch the interaction on adiabatically

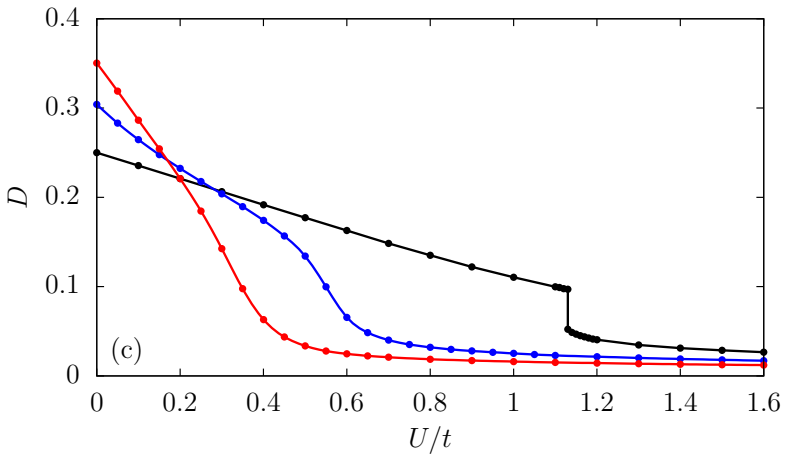
half-filling, $V = 0.5t$ and $k_B T = 0.025t$:

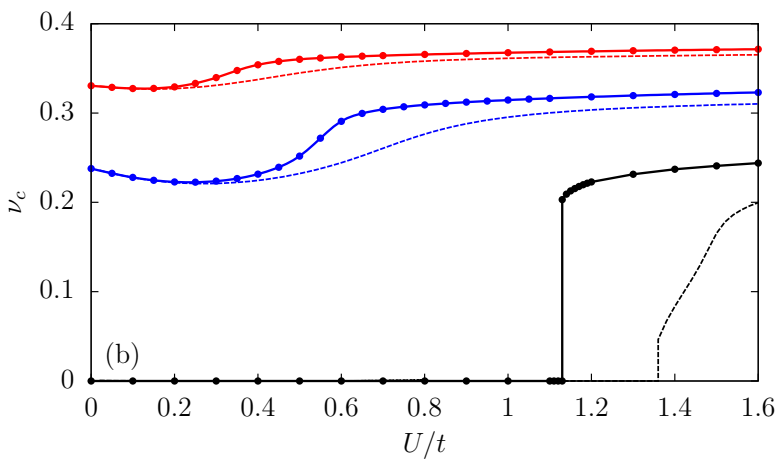


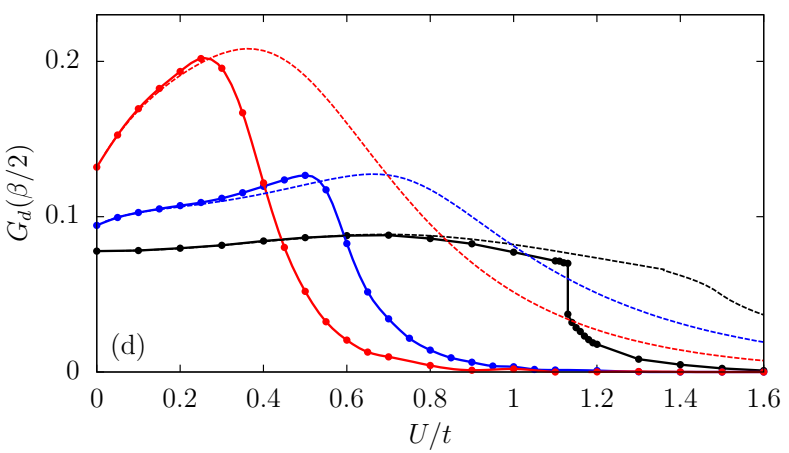
- small g: Kondo insulator phase with $\nu_d = 0$
- two SC phases that differ by the sign of the induced pairing: analogies of the 0 and π phases of SCIAM, separated by first order transition (crossover at finite T)
- reentrant behavior for small U
- interaction U promotes superconductivity





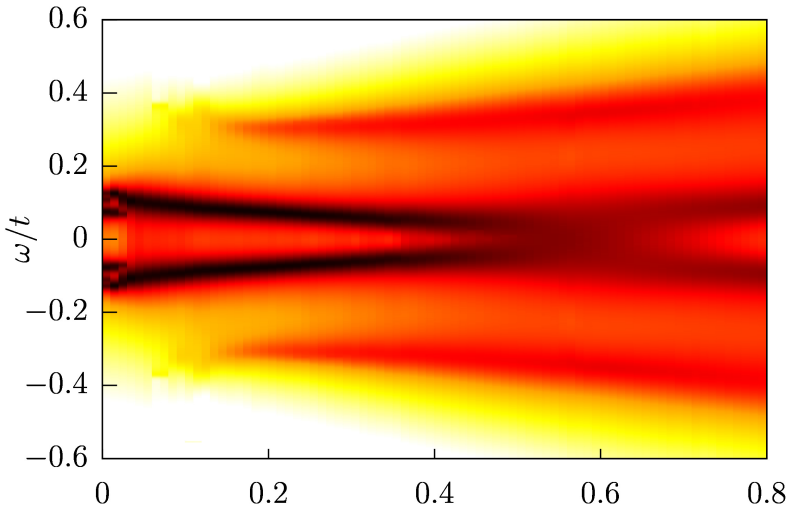


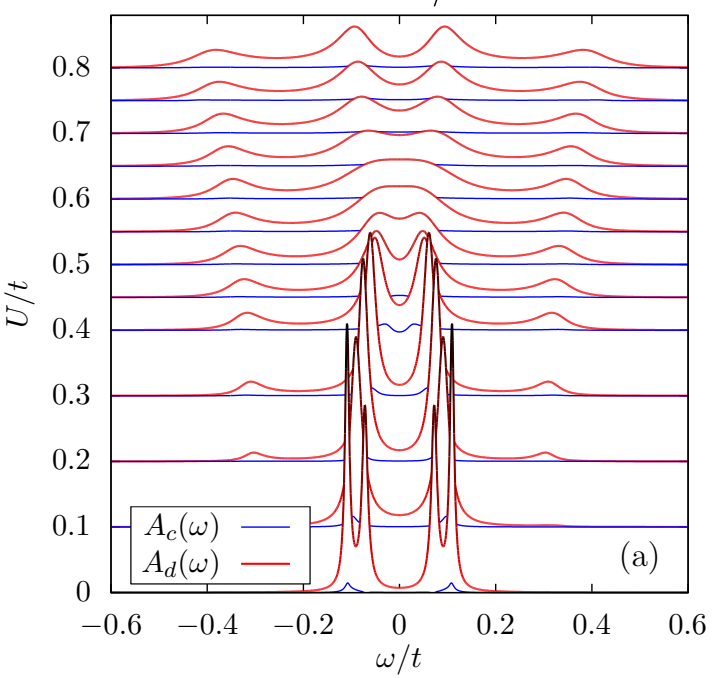


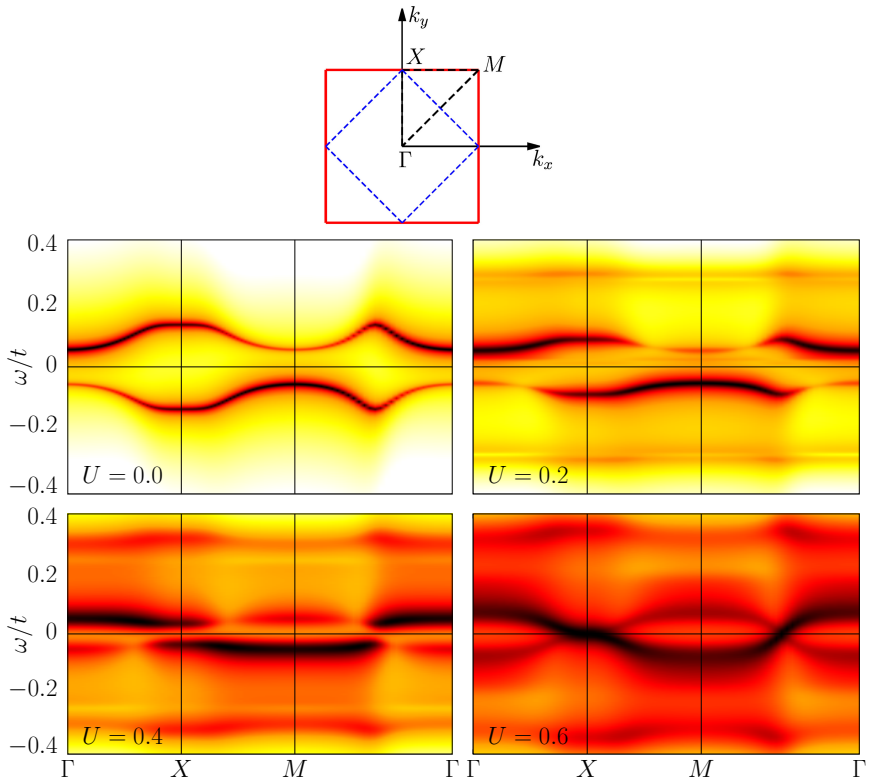


- only the induced pairing $\nu_d = \langle d_\downarrow d_\uparrow \rangle$ changes sign - phase transition is limited to the impurity band

diagonal part of the in-gap spectral function for $V = 0.5t$, $g = 5t$ and $k_B T = 0.025t$:
the Andreev bands:

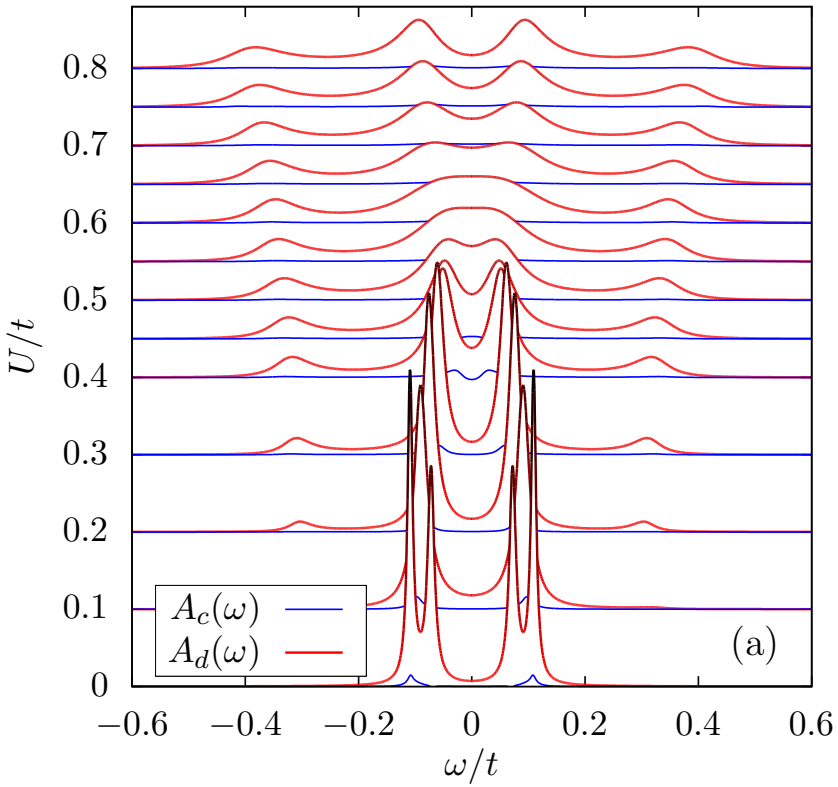




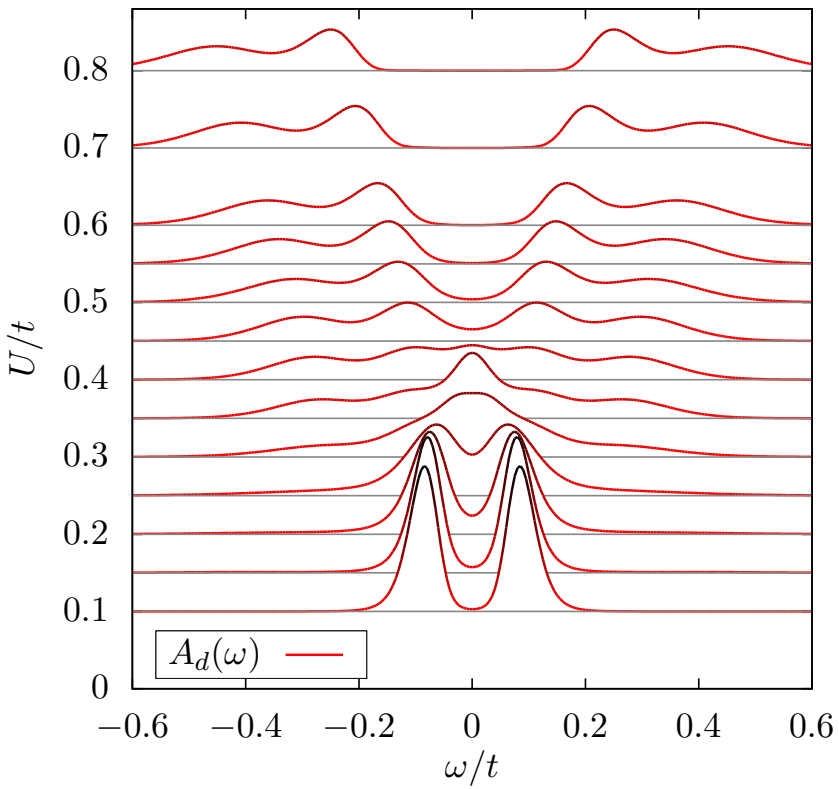


- merging of in-gap bands at $U \approx 0.6t$ where ν_d changes sign, in analogy to the $0 - \pi$ transition in the impurity model (SCIAM)
- additional band emerges at larger interaction strength

IPT:



CT-HYB + MaxEnt:

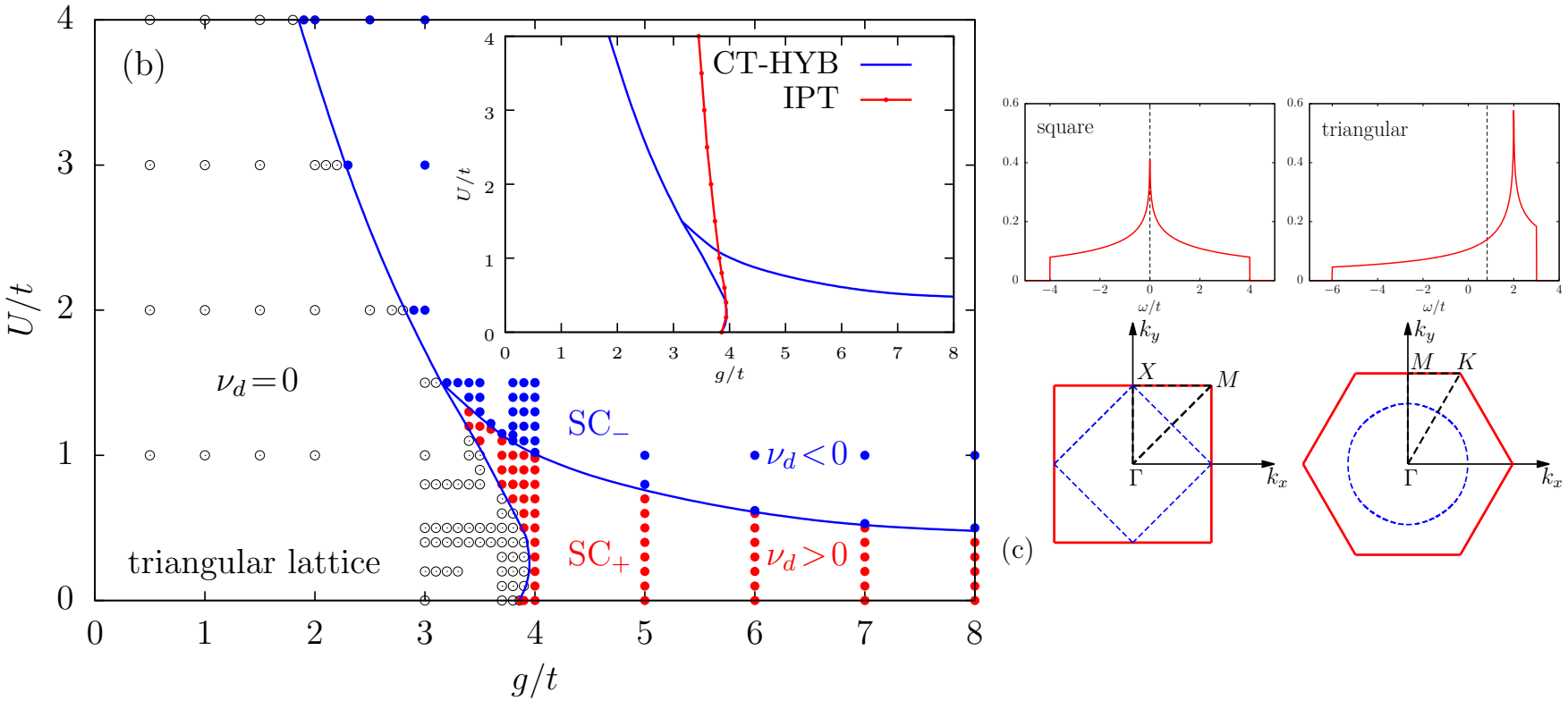


- MaxEnt data obtained using ana_cont package (1)
- Resolution was enhanced by calculating the continuation of $G_{\text{rot}}(z) = G_n(z) - G_a(z)$ and then separating the output to normal and anomalous part. Works only at half filling (2).

(1) J. Kaufmann, K. Held, arXiv:2105.11211, josefkaufmann.github.io/ana_cont

(2) E. Gull, O. Parcollet, and A. J. Millis, Phys. Rev. Lett. **110**, 216405 (2013).

half filling, $V = 0.5t$ and $k_B T = 0.025t$:



- Similar topology as for the square lattice due to local nature of DMFT.
- IPT fails to describe the SC_- phase
- Triangular lattice is not bipartite: DOS is not symmetric at half-filling. The total filling is controlled by the shift of a chemical potential which is over-estimated in IPT.

Conclusions

superconducting periodic Anderson model solved within DMFT framework:

- simple model to study the effect of the impurity band on the superconductor and vice versa
- attractive interaction in the conduction band treated using static mean-field (BCS)
- repuslive interaction in the impurity band treated using DMFT
- DMFT neglects spatial correlations whole keeping the temporal fluctuations intact
- two superconducting phases separated by a first order transition (crossover at finite T), in analogy to the 0 and π phases of the superconducting impurity Anderson model:
  - phases differ by the sign of the induced pairing,
  - in-gap bands merge at the Fermi energy around the transition point (this could explain the existence of areas of high ZBC in certain experiments),
  - phase transition happens only in the impurity band
- increasing interaction strength promotes superconductivity in the half-filled model

Future research:

- implement a solution of a renormalized effective model (the 'generalized atomic limit') we recently developed as a DMFT solver (1,2) to replace IPT
- fast efficient and reliable, allows for excessive parameter scans
- implement cluster DMFT scheme to incorporate spatial correlations in the model
- study the effects of a ferromagnetic layer on superconducting substrate

(1) V. Pokorný and M. Žonda, Phys. Rev. B **107**, 155111 (2023).

(2) M. Žonda, P. Zalom, T. Novotný, G. Loukeris, J. Bätge, and V. Pokorný, Phys. Rev. B **107**, 115407 (2023).

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Conclusions

acknowledgments:

- P. Ram, T. Novotný, M. Žonda (MFF UK, Prague, CZ)

computer resources:

- Czech National Grid Infrastructure MetaCentrum

COST action CA21144 SUPERQUMAP
(Superconducting Nanodevices and Quantum Materials for Coherent Manipulation)

reading

- V. Pokorný and P. Ram, Phys. Rev. B **104**, 155102 (2021).

Thank you for your attention.

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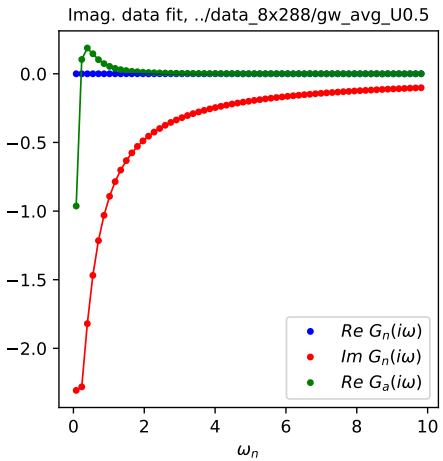
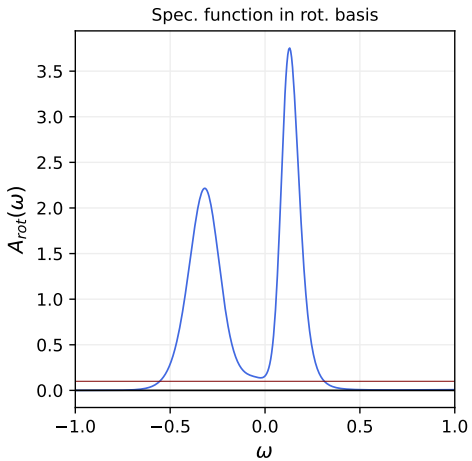
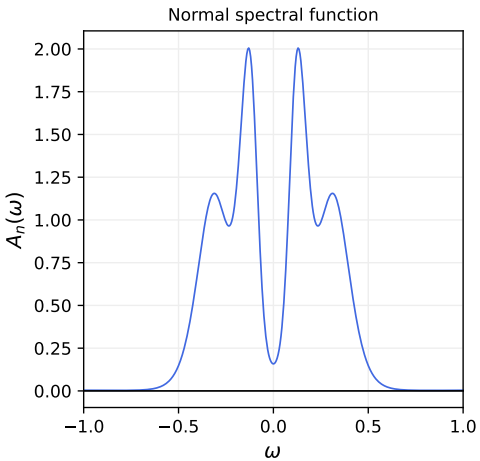
Thank you for your attention.

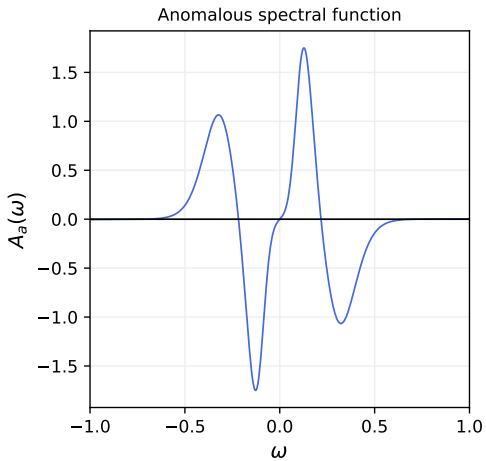
Appendix MaxEnt for matrix-valued Green functions

- Unitary transformation $T = [\sigma_x - \sigma_z]/\sqrt{2}$ diagonalizes the SCIAM Hamiltonian at half filling (1).
- Green function $G_{\mathrm{rot}}(z) = G_n(z) - G_a(z)$, ($z = \omega + i0$ or $i\omega_n$) is diagonal at half filling.
- The ABS in $G_{\mathrm{rot}}(\omega)$ are more pronounced - easier to fit using MaxEnt.
- $G_n(\omega) = [G_{\mathrm{rot}}(\omega) - G_{\mathrm{rot}}(-\omega)]/2, \qquad G_a(\omega) = -[G_{\mathrm{rot}}(\omega) + G_{\mathrm{rot}}(-\omega)]/2.$









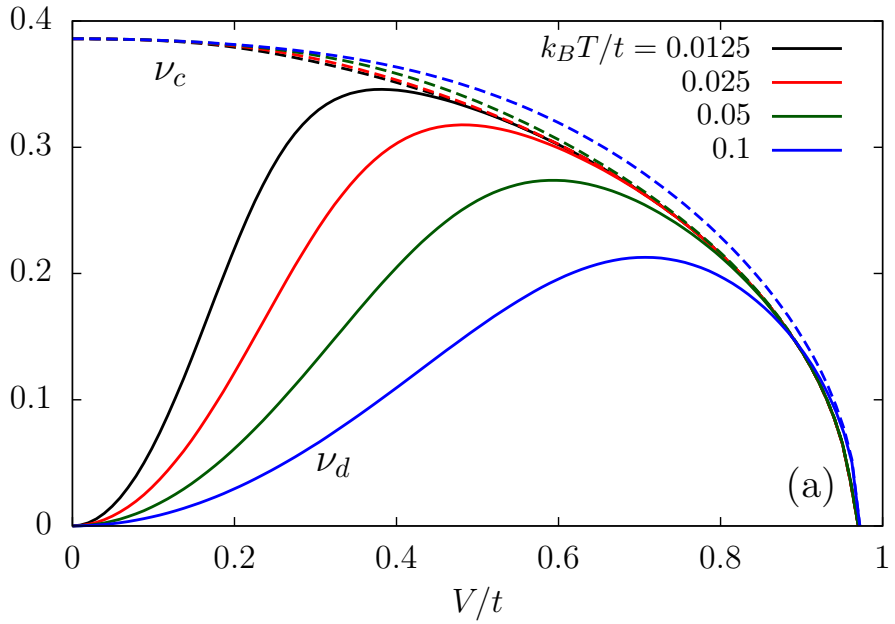
- we also obtain the anomalous spectrum
- take-home message: off-diagonal part of a matrix fermionic spectral function is not bosonic: $\mathrm{sgn}(\omega)A_a(\omega)$ is not always non-negative.
- Away from half-filling: similar, but more complex tricks are possible (2,3).

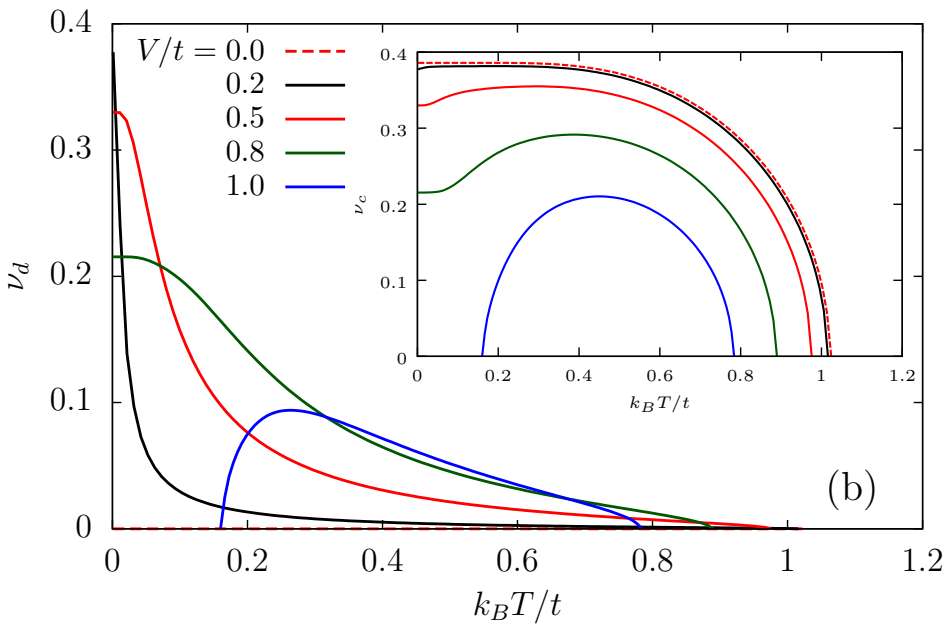
(1) P. Zalom, V. Pokorný, and T. Novotný, Phys. Rev. B **103**, 035419 (2021).

(2) Ch. Yue and P. Werner, Phys. Rev. B **108**, L220503 (2023).

(3) S. Yang, L. Du, L. Huang, arXiv:2401.00018

Non-interacting (U = 0) model

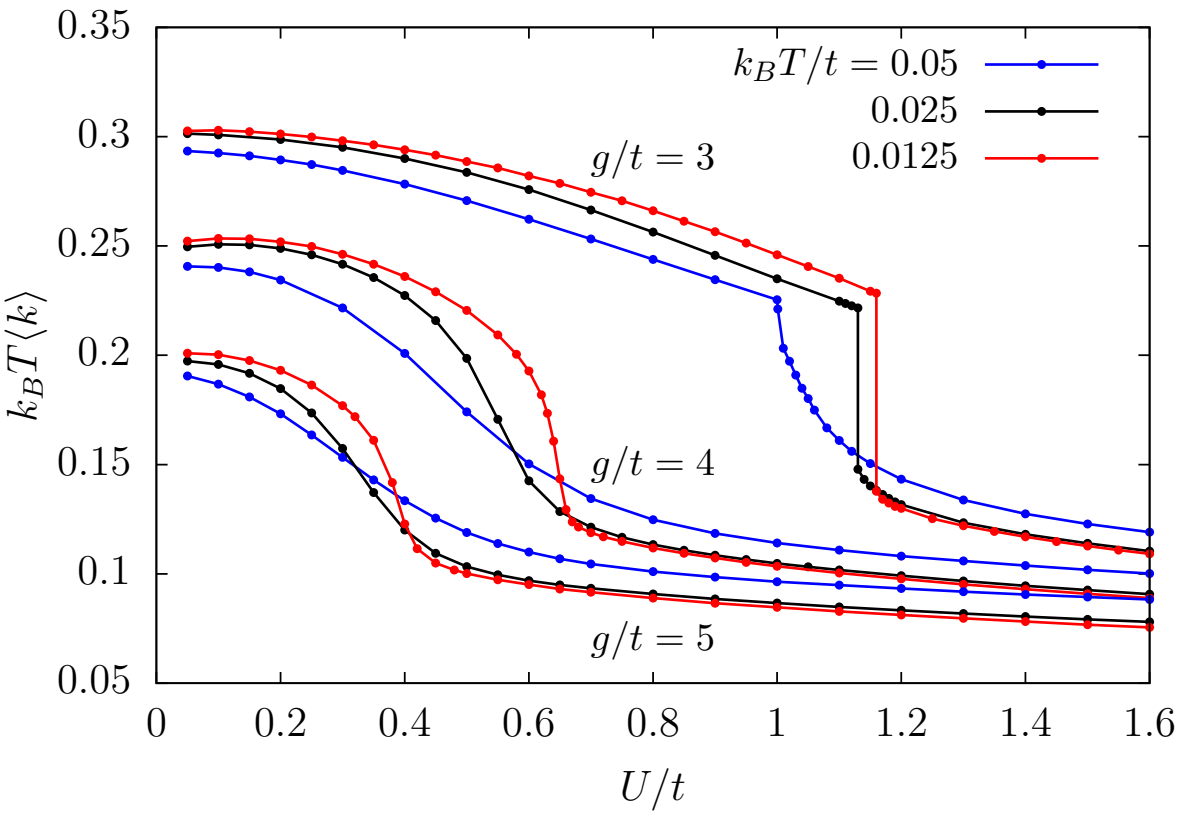




- The increasing hybridization strength promotes the induced pairing ν_d but weakens the sc correlations in the conduction band ν_c.
- Induced pairing shows reentrant behavior w.r.t. temperature at larger values of the hybridization strength.

Appendix averaged CT-HYB perturbation order

- CT-HYB performs diagrammatic expansion in hybridization term $\mathcal{H}_{\text{hyb}}$ around the atomic limit
- statistics of the expansion order k can be accumulated during the simulation
- average expansion order $\langle k \rangle = \langle \mathcal{H}_{\text{hyb}} \rangle / k_B T$ holds the information about the hybridization between the conduction and impurity bands
- temperature dependence of phase boundaries can be extracted from its behavior



(1) V. Pokorný and T. Novotný, Phys. Rev. Research **3**, 023013 (2021).