Effective low-energy models for superconducting impurity systems

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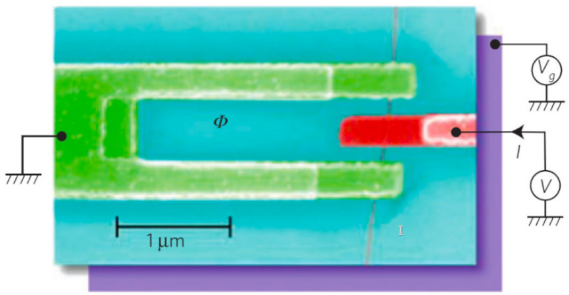
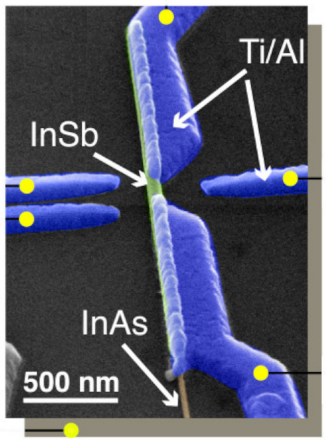
Motivation

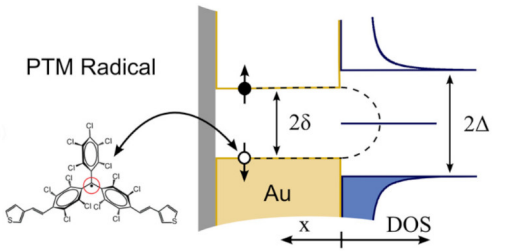
- Nanoscopic superconducting junctions
- Magnetic molecules on superconductors

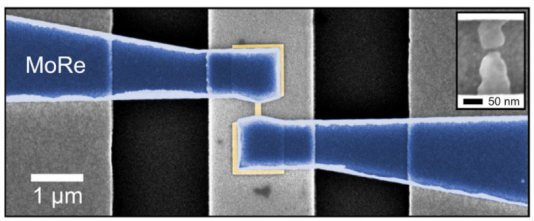


CNT, Nat. Phys. **6**, 965 (2010).



InAs nanowire, arXiv:1808.07003





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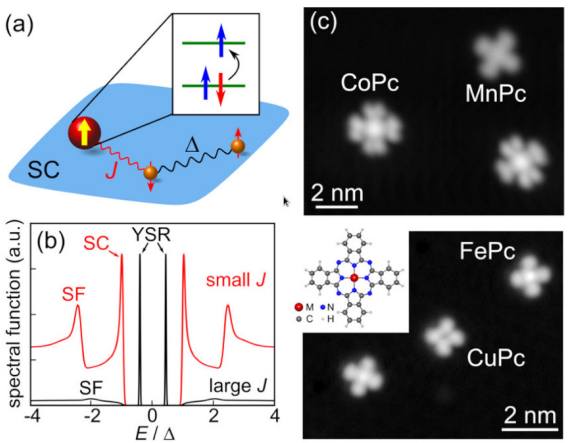
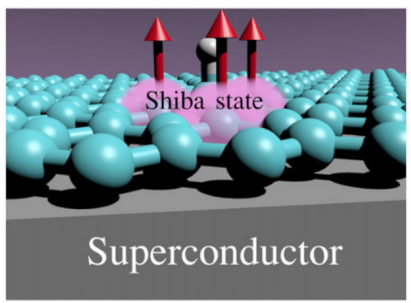
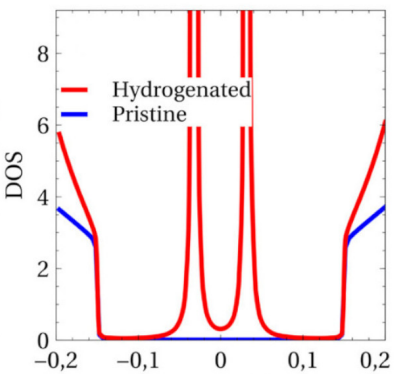


Nano Lett. **19**, 4614 (2019).



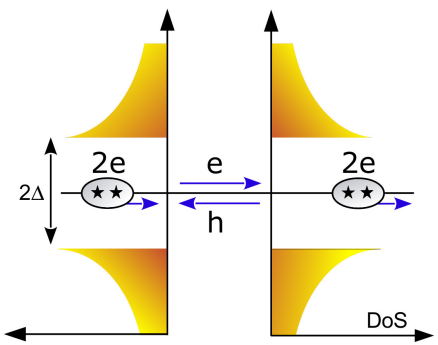


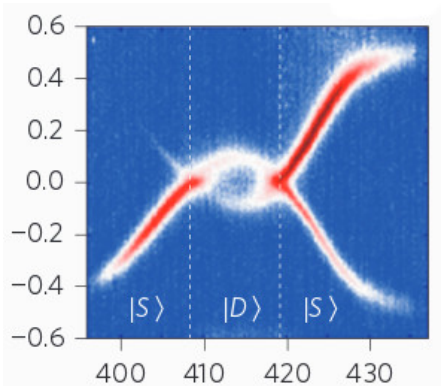
hydrogen on graphene, 2D Mater. **3**, 025001 (2016).

CNT: carbon nanotube, PTM: polychlorotriphenylmethyl, Pc: phthalocyanine

- simplest model: **single-level quantum dot connected to BCS superconducting leads**

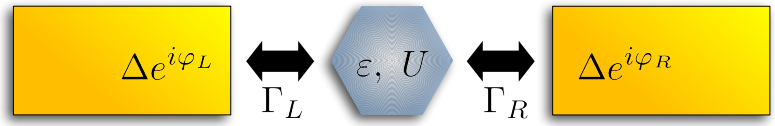
- parameters:
  - quantum dot: local energy ε and Coulomb interaction strength U
  - leads: gap width Δ and phase difference $\varphi = \varphi_L - \varphi_R$
  - coupling: tunneling rates $\Gamma_\alpha = \pi |V_\alpha|^2 \rho_\alpha$, $\alpha = L, R$
- typical values for nanowire junctions:
  - $\Delta = 100 - 1000 \mu$eV (150μeV for Al, 400μeV for NbTiN, 2.15meV for $NbSe_2$...)
  - $U \sim 10\Delta$ - dominant energy scale
  - $\Gamma \sim \Delta$ (typically, but varies much between setups)
  - $\varphi \in (0, 2\pi)$ can be tuned by magnetic flux in SQUID setups, zero otherwise
- most of the properties are governed by the behavior of the in-gap, **Andreev bound states** (ABS) (also known as Yu-Shiba-Rusinov, YSR states)





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

- crossing of the Andreev bound states at the Fermi energy: singlet-doublet ($0 - \pi$) **impurity quantum phase transition**



- such system can be often reliably described using superconducting Anderson impurity model

$$\mathcal{H} = \mathcal{H}_d + \sum_{\alpha} (\mathcal{H}_c^{\alpha} + \mathcal{H}_{\text{hyb}}^{\alpha}), \quad \alpha = L, R$$

- single-level quantum dot (w/o magnetic field)

$$\mathcal{H}_d = \varepsilon \sum_{\sigma} d_{\sigma}^{\dagger} d_{\sigma} + U \left(d_{\uparrow}^{\dagger} d_{\uparrow} - 1/2 \right) \left(d_{\downarrow}^{\dagger} d_{\downarrow} - 1/2 \right)$$

(local energy shifted by $U/2$ so $\varepsilon = 0$ corresponds to a half-filled impurity)

- superconducting leads

$$\mathcal{H}_c^{\alpha} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} c_{\alpha\mathbf{k}\sigma}^{\dagger} c_{\alpha\mathbf{k}\sigma} - \Delta \sum_{\mathbf{k}} (e^{i\varphi_{\alpha}} c_{\alpha\mathbf{k}\uparrow}^{\dagger} c_{\alpha-\mathbf{k}\downarrow}^{\dagger} + \text{H.c.})$$

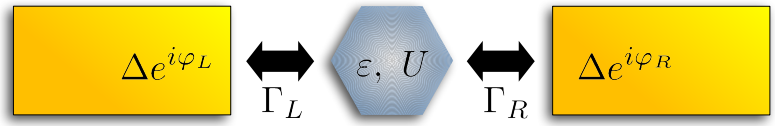
$\Delta e^{i\varphi_{\alpha}} = g \langle c_{\alpha-\mathbf{k}\downarrow} c_{\alpha\mathbf{k}\uparrow} \rangle$ is the (complex) BCS order parameter

- coupling terms

$$\mathcal{H}_{\text{hyb}}^{\alpha} = -\sum_{\mathbf{k}\sigma} (V_{\alpha\mathbf{k}} c_{\alpha\mathbf{k}\sigma}^{\dagger} d_{\alpha\sigma} + \text{H.c.}), \qquad \Gamma_{\alpha} = \pi |V_{\alpha}|^2 \rho_{\alpha}$$

V. Meden, J. Phys. Condens. Matter **31**, 163001 (2019).

D. J. Luitz, F. F. Assaad, T. Novotný, C. Karrasch, and V. Meden, Phys. Rev. Lett. **108**, 227001 (2012).



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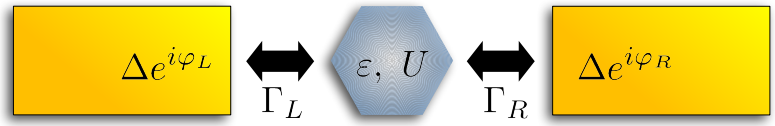

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- infinite superconducting gap, $\Delta \to \infty$ after we take the infinite-bandwidth limit (otherwise we decouple the leads and end up with a trivial model)
- exactly solvable atomic model (4×4 matrix in $|0\rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$, $|\uparrow\downarrow\rangle$ basis)

$$\mathcal{H}_\infty = \varepsilon \sum_\sigma d_\sigma^\dagger d_\sigma - \left(\Gamma_\varphi d_\uparrow^\dagger d_\downarrow^\dagger + \text{H.c.}\right) + U\left(d_\uparrow^\dagger d_\uparrow - 1/2\right)\left(d_\downarrow^\dagger d_\downarrow - 1/2\right)$$

where $\Gamma_\varphi = \Gamma_L e^{i\varphi_L} + \Gamma_R e^{i\varphi_R}$

- spectrum consists of two spin-singlets and one spin-doublet
- crossing of the ABS states at the Fermi energy marks the singlet-doublet ($0 - \pi$) impurity quantum phase transition at $U = 2\sqrt{\Gamma_\varphi^2 + \varepsilon^2}$.

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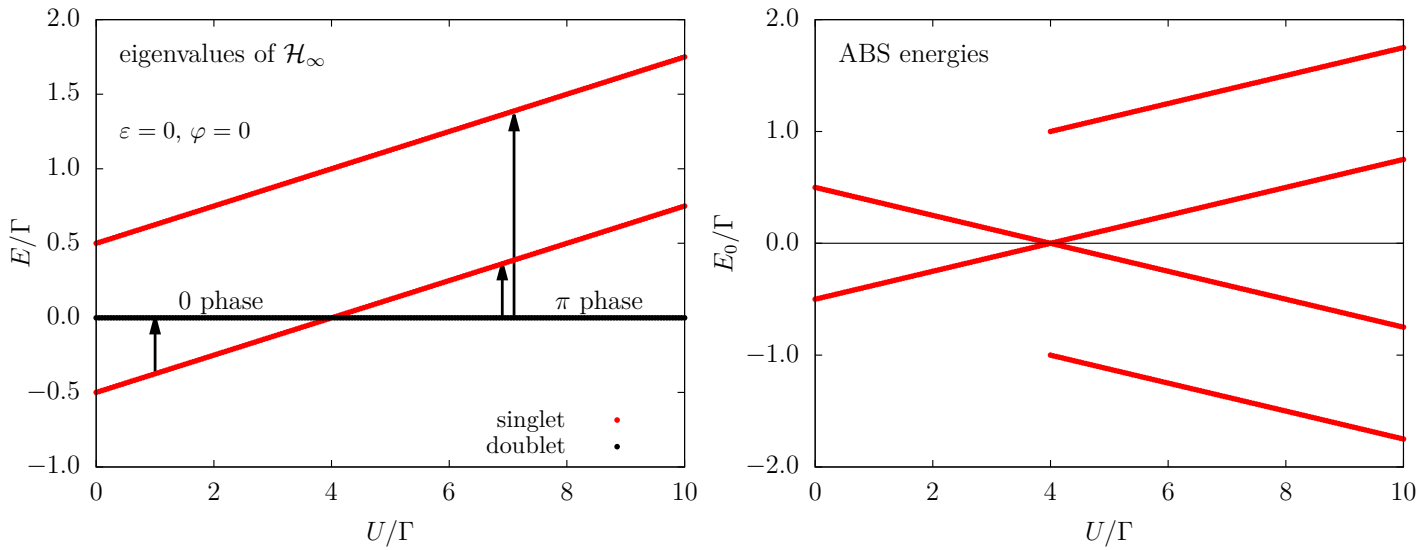

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solvers for the superconducting Anderson impurity model

- diagrammatic expansion techniques (Hartree-Fock, second-order PT...) - fast and simple, but bound to the singlet (0) phase only
- effective models (superconducting atomic limit, zero bandwidth limit) - often qualitatively correct, but quantitatively off (even by orders of magnitude)
- numerical renormalization group (NRG) - usually the method of choice for one or two correlated levels, cannot be employed for more complicated systems
- CT-HYB quantum Monte Carlo - flexible method, can be employed for various geometries and multi-dot setups, but
  - formulated in imaginary-time formalism - dynamical sign problem prohibits real-time implementations (exceptions exist, i.e., the inchworm algorithm)
  - bound to finite temperatures ($k_B T \gtrsim 0.01\Delta$)
  - no direct access spectral functions / Andreev bound state energies

- Can we obtain the ABS energies from CT-HYB QMC without analytic continuation?
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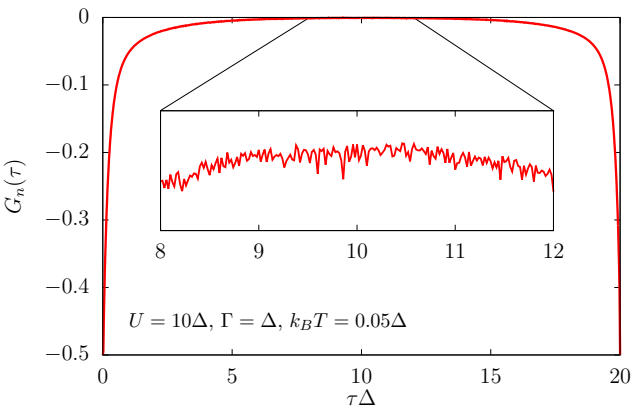
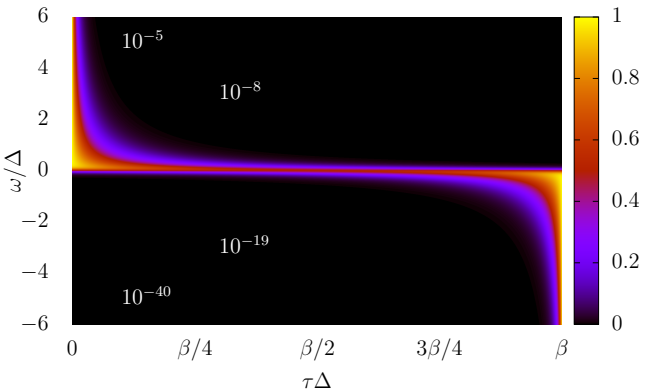
- Can we obtain the ABS energies from CT-HYB QMC without analytic continuation?
- Is it possible to modify the effective models to give quantitatively reasonable solutions?

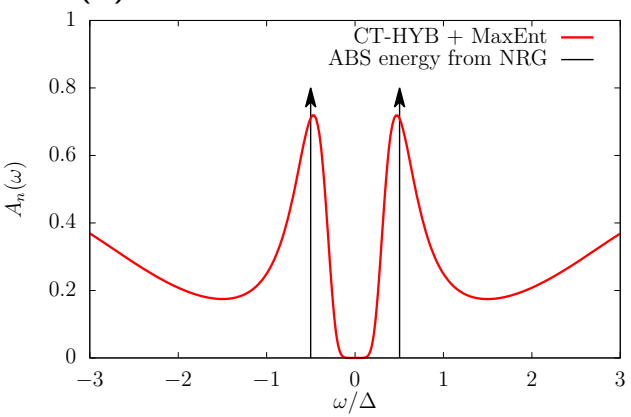
- CT-HYB Green function is calculated in imaginary time, no direct access to spectral functions/ABS frequencies
- analytic continuation $i\tau \rightarrow \omega$ of noisy data is an ill-defined problem (there is an infinite number of spectral functions $A(\omega)$ which correspond to the same noisy $G(\tau)$)
- $G(\tau)$ 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)







- lesson from the superconducting atomic limit: the low-energy ($|\omega| < \Delta$) part of the spectral function (i.e., Andreev bound states) dictates most of the properties of these systems
- we might not need the whole spectral function

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

- interacting Green function

$$G^{-1}(\omega) = G_0^{-1}(\omega) - \Sigma(\omega) = \begin{pmatrix} \omega[1+s(\omega)] - \varepsilon - \Sigma_n(\omega) & \Delta_\varphi(\omega) - \Sigma_a(\omega) \\ \Delta_\varphi(\omega) - \Sigma_a(\omega) & \omega[1+s(\omega)] + \varepsilon + \Sigma_n^*(-\omega) \end{pmatrix}$$

- we expand the ω-dependent terms around $\omega = 0$ (Fermi energy):

$$s(\omega) = \frac{\Gamma}{\Delta} + \frac{\Gamma}{2\Delta^3}\omega^2 + \mathcal{O}(\omega^4), \qquad \Delta_\varphi(\omega) = \Gamma_\varphi + \frac{\Gamma_\varphi}{2\Delta^2}\omega^2 + \mathcal{O}(\omega^4),$$

$$\Sigma_j(\omega) = \Sigma_j(0) + \omega \frac{\partial \Sigma_j}{\partial \omega}\Big|_0 + \omega^2 \frac{1}{2} \frac{\partial^2 \Sigma_j}{\partial \omega^2}\Big|_0 + \mathcal{O}(\omega^3), \qquad j = n, a$$

- low-energy model: non-interacting atomic limit with renormalized parameters + correction for incoherent states $\mathcal{C}(\omega)$ ($\tilde{\Sigma}_j(0)$ is just a real number)

$$G^{-1}(\omega) = Z^{-1} \begin{pmatrix} \omega - \tilde{\varepsilon} - \tilde{\Sigma}_n(0) & \tilde{\Gamma}_\varphi - \tilde{\Sigma}_a(0) \\ \tilde{\Gamma}_\varphi - \tilde{\Sigma}_a(0) & \omega + \tilde{\varepsilon} + \tilde{\Sigma}_n(0) \end{pmatrix} + \mathcal{C}(\omega) = Z^{-1}[\tilde{G}^{-1}(\omega) + \tilde{\mathcal{C}}(\omega)]$$

- renormalization factor: renormalized parameters:

$$Z = \left(1 + \frac{\Gamma}{\Delta} - \frac{\partial \Sigma_n}{\partial \omega}\Big|_0\right)^{-1}, \qquad \tilde{\varepsilon} = Z\varepsilon, \quad \tilde{\Gamma}_\varphi = Z\Gamma_\varphi, \quad \tilde{\Sigma}(0) = Z\Sigma(0)$$

- ABS energies: poles of the Green function, zeros of $\det G^{-1}(\omega)$:

$$E_0 = \pm\sqrt{[\tilde{\varepsilon} + \tilde{\Sigma}_n(0)]^2 + [\tilde{\Gamma}_\varphi - \tilde{\Sigma}_a(0)]^2} = \pm Z\sqrt{[\varepsilon + \Sigma_n(0)]^2 + [\Gamma_\varphi - \Sigma_a(0)]^2}.$$

- quantum critical point is marked by the crossing of the ABS: $E_0 = 0$

$$\Gamma_\varphi - \Sigma_a(0) = \pm[\varepsilon + \Sigma_n(0)]$$

($\pm$ sign reflects the electron-hole symmetry $\varepsilon \to -\varepsilon$)

- its position depends only on the model parameters and self-energy at zero
- unfortunately, this model always gives only two ABS energies, even in the π phase
- model can be systematically improved by considering more terms in the expansion:

$$ZG_n^{-1} = -\frac{\tilde{\Sigma}_n''(0)}{2}\omega^2 + \omega - \tilde{\varepsilon} - \tilde{\Sigma}_n(0),$$

$$ZG_a^{-1} = \frac{1}{2}\left(\frac{\tilde{\Gamma}_\varphi}{\Delta^2} - \tilde{\Sigma}_a''(0)\right)\omega^2 + \tilde{\Gamma}_\varphi - \tilde{\Sigma}_a(0)$$

we get a 4th order equation for ABS energies, but two always lie above the gap: no help

- We need to supply our model with the real-frequency derivatives of the self-energy at zero
- 1. Can we use CT-HYB data?
- 2. Can we use effective models to provide self-energy?

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- CT-HYB gives us self-energy in imaginary Matsubara frequencies $\omega_n = (2n+1)\pi k_B T$
- analytic continuation $\omega_n \to \omega + i0$: problematic
- we don't need the whole self-energy, only the value and derivatives at $\omega = 0$ (all real)

- Cauchy-Riemann equations ($z = \omega + i\omega_n$):

$$\frac{\partial \operatorname{Re}\Sigma_j(z)}{\partial \omega} = \frac{\partial \operatorname{Im}\Sigma_j(z)}{\partial \omega_n},$$
$$\frac{\partial \operatorname{Re}\Sigma_j(z)}{\partial \omega_n} = -\frac{\partial \operatorname{Im}\Sigma_j(z)}{\partial \omega}.$$

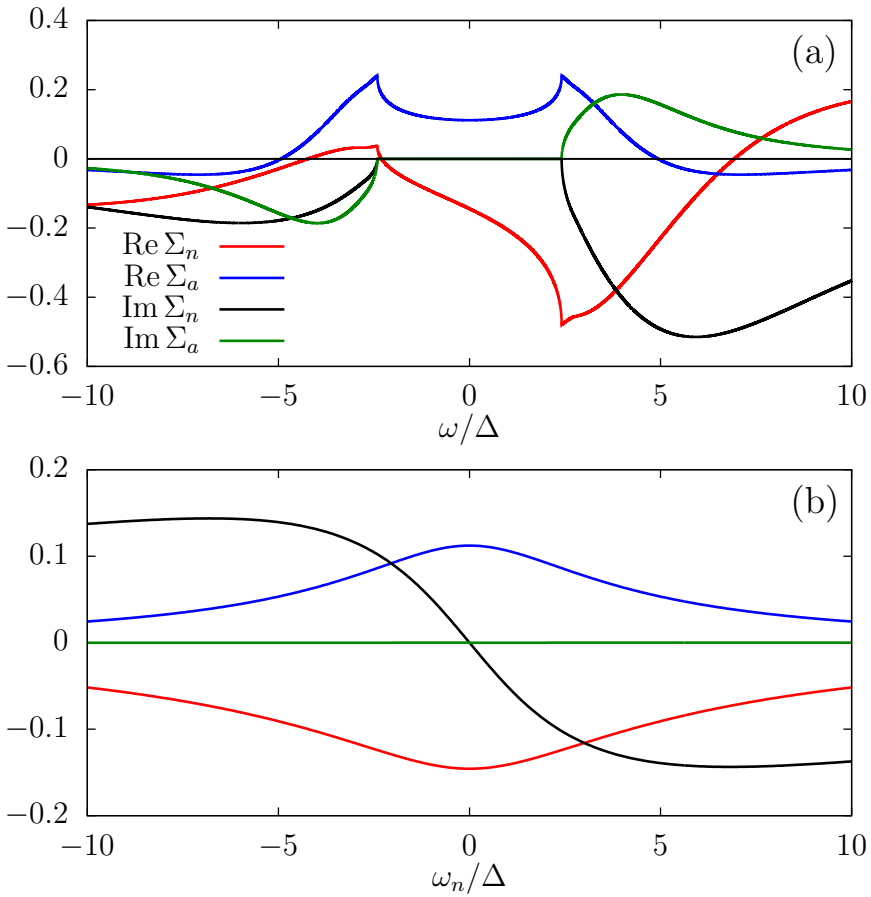
- higher derivatives:

$$\frac{\partial^2 \operatorname{Re}\Sigma_j(z)}{\partial \omega^2} = -\frac{\partial^2 \operatorname{Re}\Sigma_j(z)}{\partial \omega_n^2},$$
$$\frac{\partial^3 \operatorname{Re}\Sigma_j(z)}{\partial \omega^3} = -\frac{\partial^3 \operatorname{Im}\Sigma_j(z)}{\partial \omega_n^3},$$

etc . . .

- allow us to estimate the derivatives along real axis from imaginary-frequency data
- numerical derivative of stochastic function: requires high-quality QMC data

illustration: 2PT solution at $T = 0$:



- can we somehow employ the knowledge of the exact solution in the atomic limit?
- low-energy limit of the non-interacting Green function: non-interacting atomic model

$$G_0^{-1}(\omega) = \begin{pmatrix} \omega[1+s(\omega)] - \varepsilon & \Delta_\varphi(\omega) \\ \Delta_\varphi(\omega) & \omega[1+(\omega)] + \varepsilon \end{pmatrix} = Z^{-1} \begin{pmatrix} \omega - \tilde{\varepsilon} & \tilde{\Gamma}_\varphi \\ \tilde{\Gamma}_\varphi & \omega + \tilde{\varepsilon} \end{pmatrix} + \mathcal{C}(\omega)$$

$Z^{-1} = (1 + \Gamma/\Delta), \quad \tilde{\varepsilon} = Z\varepsilon, \quad \tilde{\Gamma}_\varphi = Z\Gamma_\varphi$

- it corresponds to non-interacting atomic Hamiltonian

$$\tilde{\mathcal{H}}_{0,\infty} = \tilde{\varepsilon} \sum_\sigma f_\sigma^\dagger f_\sigma - \left(\tilde{\Gamma}_\varphi f_\uparrow^\dagger f_\downarrow^\dagger + \text{H.c.} \right)$$

- we know the exact solution for the interacting problem: let us add the interaction part:

$$\tilde{\mathcal{H}}_{\infty} = \tilde{\varepsilon} \sum_\sigma f_\sigma^\dagger f_\sigma - \left(\tilde{\Gamma}_\varphi f_\uparrow^\dagger f_\downarrow^\dagger + \text{H.c.} \right) + \tilde{U} \left(f_\uparrow^\dagger f_\uparrow - 1/2 \right) \left(f_\downarrow^\dagger f_\downarrow - 1/2 \right)$$

- this way we could replace the exact self-energy by the scaled self-energy in the atomic limit

$$\Sigma(\omega; \Delta, \varphi, \varepsilon, \Gamma, U) \approx Z^{-1} \Sigma_\infty(\omega; \Delta, \varphi, \tilde{\varepsilon}, \tilde{\Gamma}, \tilde{U})$$

- problem: we don't know the relation between U and $\tilde{U}$

- can we somehow employ the knowledge of the exact solution in the atomic limit?
- low-energy limit of the non-interacting Green function: non-interacting atomic model

$$G_0^{-1}(\omega) = \begin{pmatrix} \omega[1+s(\omega)] - \varepsilon & \Delta_\varphi(\omega) \\ \Delta_\varphi(\omega) & \omega[1+(\omega)] + \varepsilon \end{pmatrix} = Z^{-1} \begin{pmatrix} \omega - \tilde{\varepsilon} & \tilde{\Gamma}_\varphi \\ \tilde{\Gamma}_\varphi & \omega + \tilde{\varepsilon} \end{pmatrix} + \mathcal{C}(\omega)$$

$Z^{-1} = (1 + \Gamma/\Delta), \quad \tilde{\varepsilon} = Z\varepsilon, \quad \tilde{\Gamma}_\varphi = Z\Gamma_\varphi$

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- problem: we don't know the relation between U and $\tilde{U}$

- hint: the leading order asymptotics of the GAL Green function w/o the correction $\mathcal{C}$:

$$G_0(\omega) = Z \begin{pmatrix} \omega - \tilde{\varepsilon} & \tilde{\Gamma}_\varphi \\ \tilde{\Gamma}_\varphi & \omega + \tilde{\varepsilon} \end{pmatrix}^{-1} = \frac{Z}{\omega} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \mathcal{O}(\omega^{-2})$$

- it describes particles with non-cannonical anticommutation relations:

$$\{d_\alpha, d_\beta^\dagger\} = Z\delta_{\alpha\beta}$$

  i.e., quasiparticle with weight $Z = (1 + \Gamma/\Delta)^{-1} \leq 1$

- we can formally rescale the operators so they obey standard commutation relations:

$$f_\alpha = \sqrt{Z} d_\alpha, \qquad f_\alpha^\dagger = \sqrt{Z} d_\alpha^\dagger$$

  and we obtain an atomic model with correct asymptotic behavior:

$$\tilde{\mathcal{H}}_\infty = \tilde{\varepsilon} \sum_\sigma f_\sigma^\dagger f_\sigma - \left(\tilde{\Gamma}_\varphi f_\uparrow^\dagger f_\downarrow^\dagger + \text{H.c.} \right) + \tilde{U} \left(f_\uparrow^\dagger f_\uparrow - 1/2 \right) \left(f_\downarrow^\dagger f_\downarrow - 1/2 \right)$$

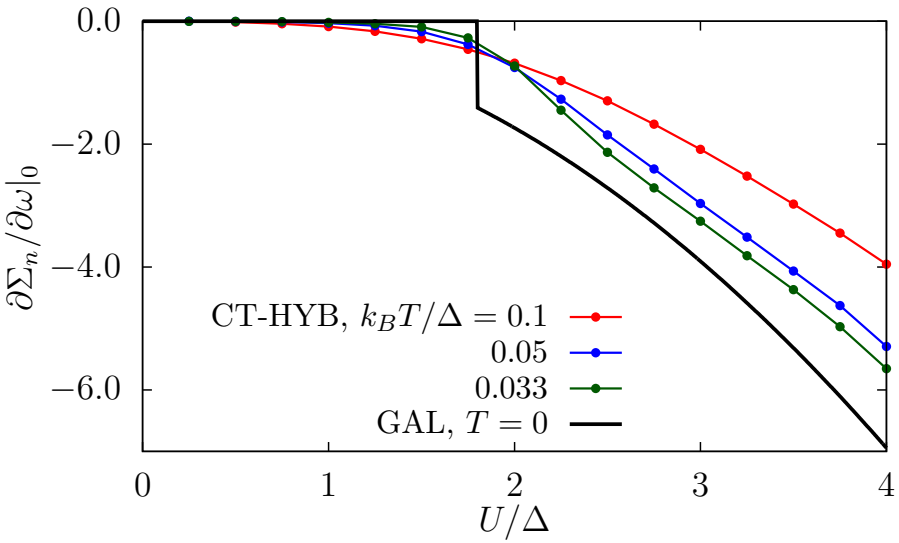
- this 'hand-waving' argument gives us a recipe how to rescale the parameters:

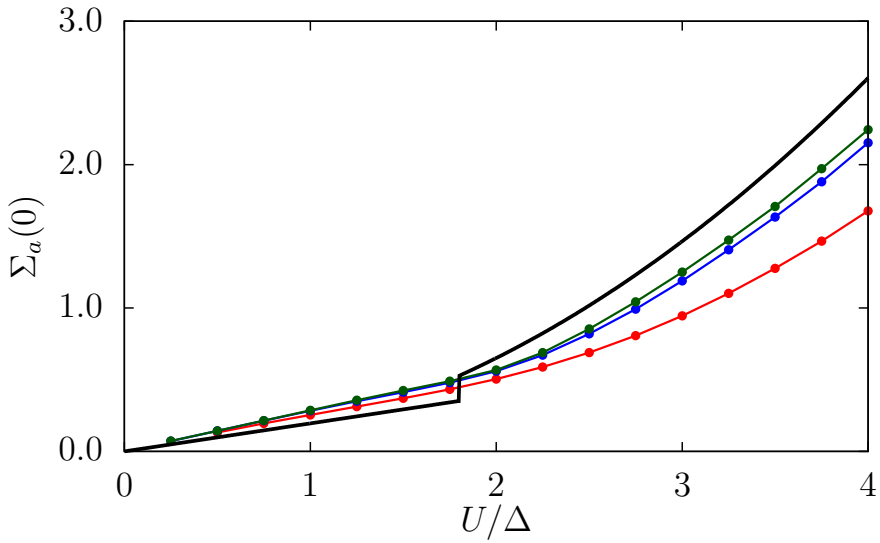
$$Z^{-1} = (1 + \Gamma/\Delta), \quad \tilde{\varepsilon} = Z\varepsilon, \quad \tilde{\Gamma}_\varphi = Z\Gamma_\varphi, \quad \tilde{U} = Z^2 U$$

- the band correction $\mathcal{C}$ corrects the asymptotic behavior of the GAL Green function

- how good is this approximation?
- we compare $\Sigma(\omega; \Delta, \varphi, \varepsilon, \Gamma, U)$ vs. $Z^{-1}\Sigma_\infty(\omega; \Delta, \varphi, Z\varepsilon, Z\Gamma, Z^2U)$

$\Gamma = 0.6\Delta$, $\varphi = 0$, half-filling ($\Sigma_n(0) = U/2$), no mag. field ($\partial\Sigma_a/\partial\omega|_0 = 0$)





We have two options how to feed our low-energy model with self-energy:

- CT-HYB self-energy
- atomic limit with properly rescaled parameters

- how good is this approximation?
- we compare $\Sigma(\omega; \Delta, \varphi, \varepsilon, \Gamma, U)$ vs. $Z^{-1}\Sigma_\infty(\omega; \Delta, \varphi, Z\varepsilon, Z\Gamma, Z^2U)$

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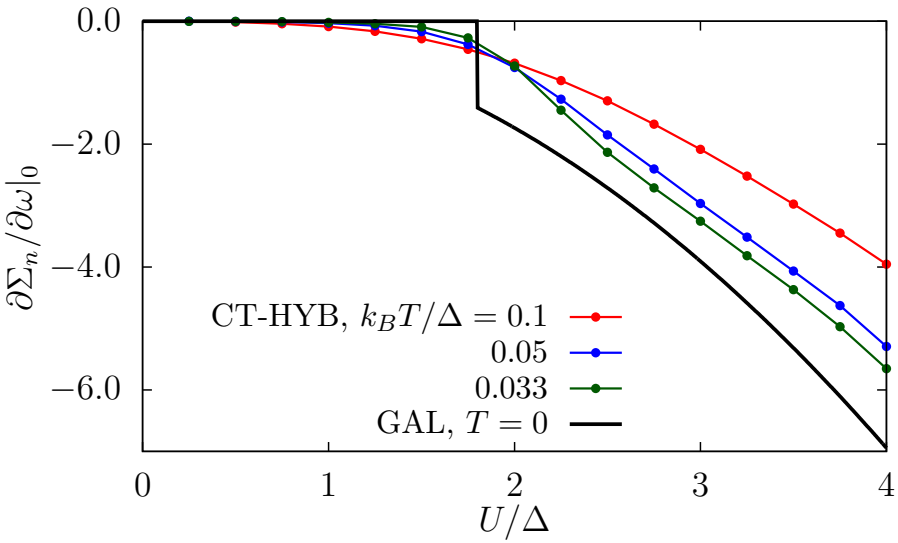

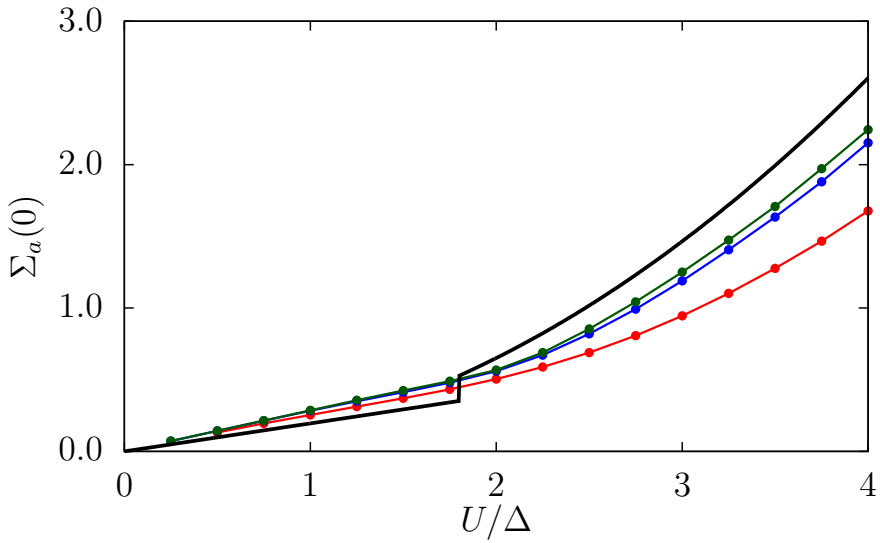

We have two options how to feed our low-energy model with self-energy:

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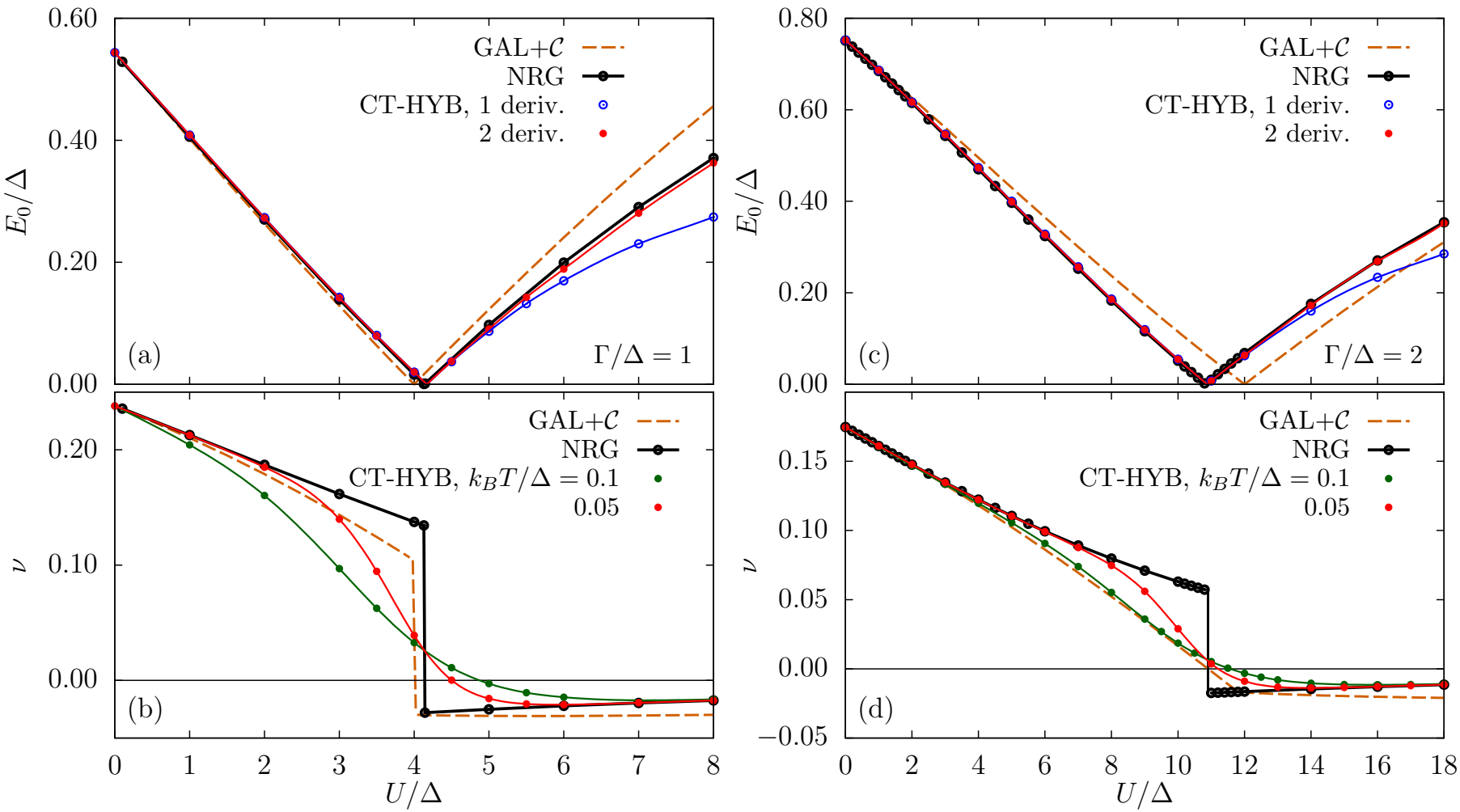
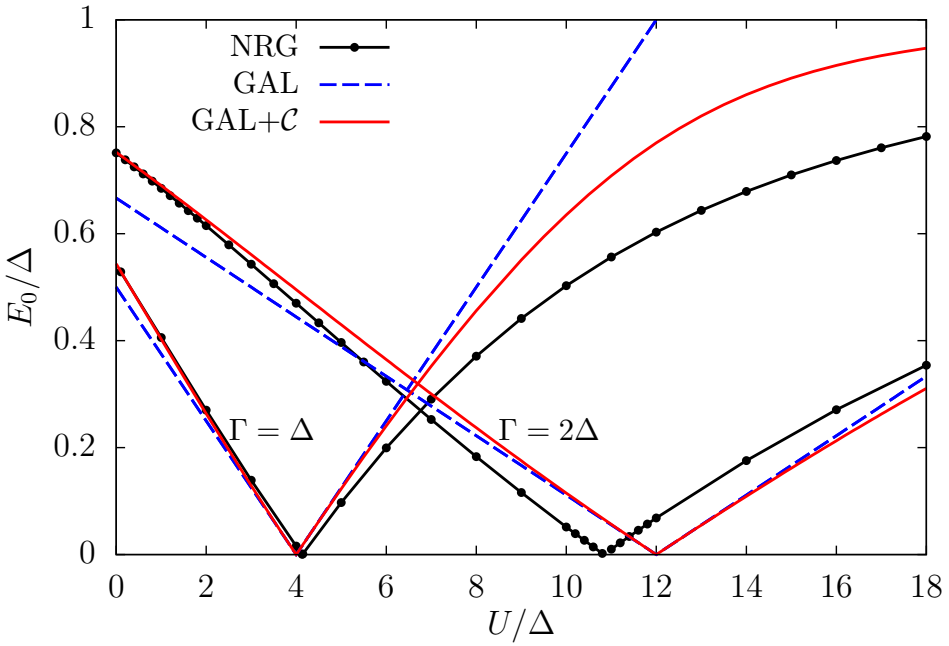
- interaction strength U is usually the largest energy scale ($U \sim 10\Delta$)
- we compare the CT-HYB and GAL results w.r.t. 'numerically exact' NRG data

half-filling, $\varphi = 0$, $\Gamma = \Delta$: $\Gamma = 2\Delta$:



- band correction $\mathcal{C}$ contains all the higher terms of the expansion of the hybridization terms $s(\omega)$ and $\Delta_\varphi(\omega)$
- results of GAL with/without the correction vs NRG:

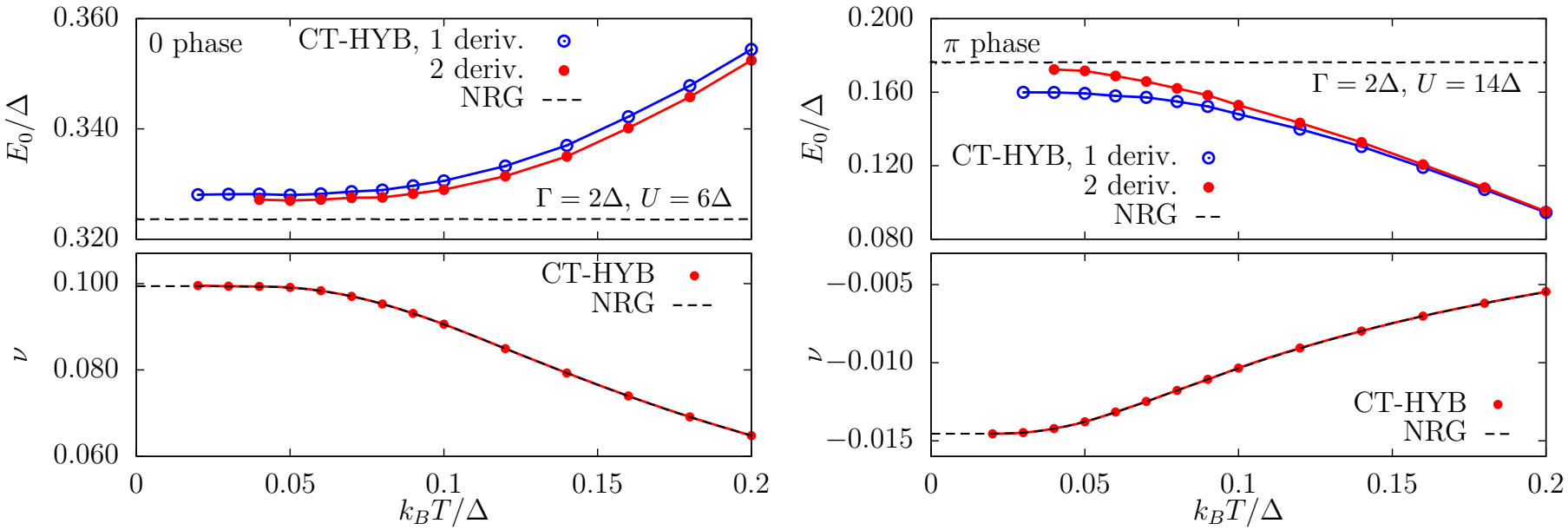


such correction is important:

- keeps the ABS energies below Δ
- guarantees the exact solution for $U = 0$
- restores the continuous part of the spectral function and provides the correct asymptotics for the Green function
- corrects the behavior of the Josephson current (1)

(1) V. Pokorný and M. Žonda, arXiv:2209.11868 (2022).

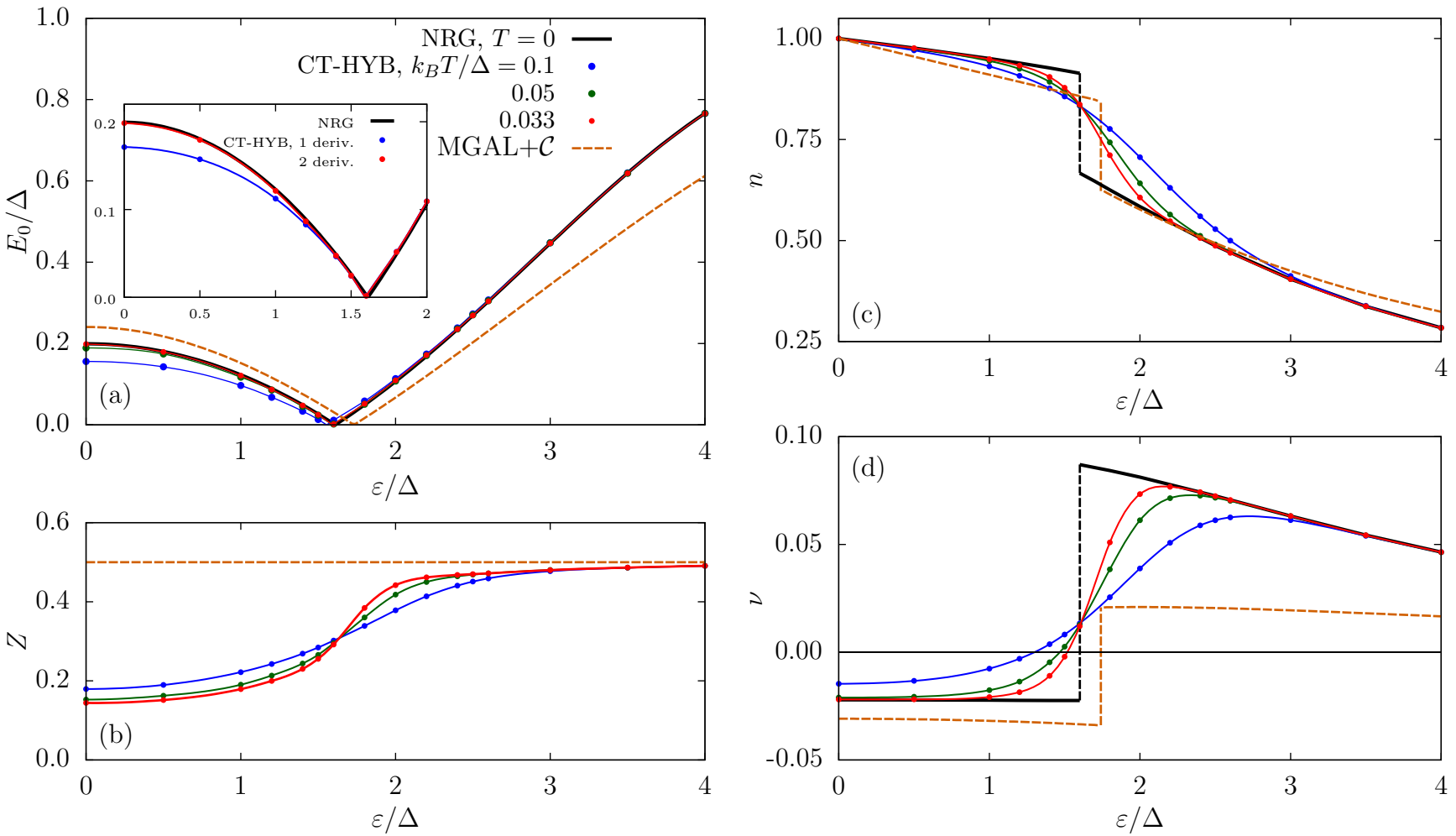
- CPU time in CT-HYB simulation scales as $t_c \sim T^{-2}$ - low-T region is inaccessible
- we should look into the convergence w.r.t. decreasing temperature



- ABS energy changes slowly below $k_B T \sim 0.1\Delta$, very little below $k_B T \sim 0.05\Delta$
- slight systematic disagreement between CT-HYB and QMC (below 2%) at low-T
- integral values (e.g. induced pairing $\nu = \langle d_\downarrow d_\uparrow \rangle$) match remarkably well (up to four decimal places)
- ABS energy from NRG is T-independent (1), CT-HYB predicts the change in agreement with some other results (2-3)

(1) R. Žitko, Phys. Rev. B **93**, 195125 (2016).
(2) C. Liu, Y. Huang, Y. Chen, and C. S. Ting, Phys. Rev. B **99**, 174502 (2019).
(3) V. Janiš and J. Yan, AIP Adv. **12**, 035139 (2022).

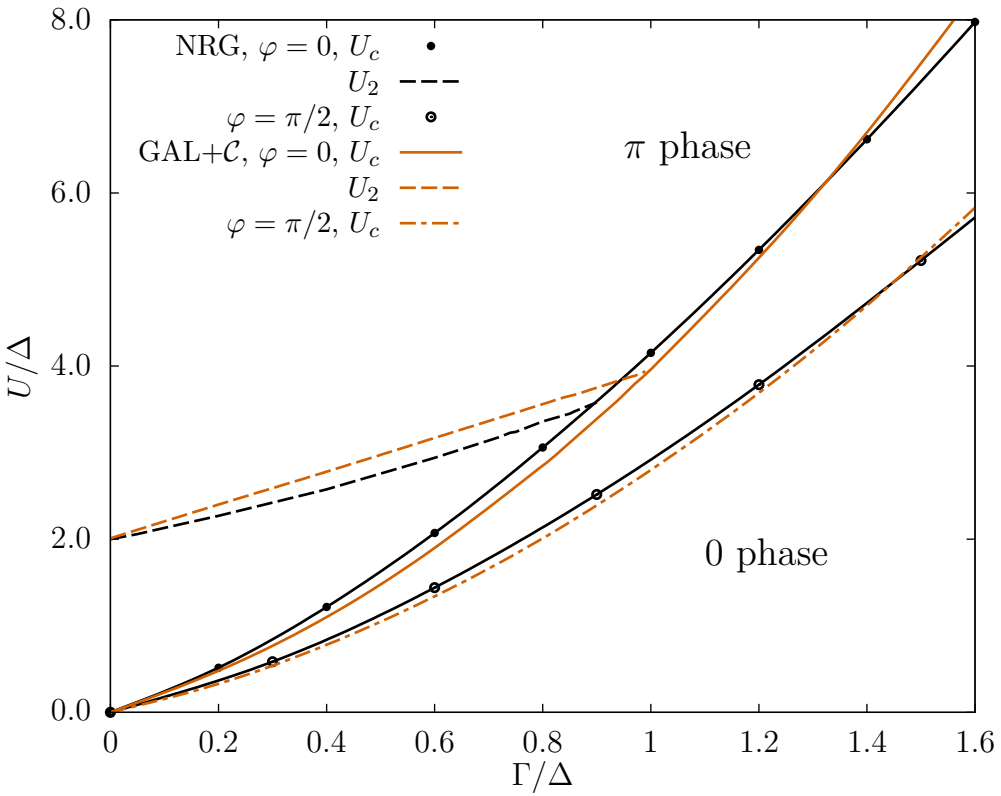
- GAL without corrections does not provide reasonable results away from half-filling
- a correction to the value of the energy level ε was obtained by fitting the 'numerically exact' NRG data (1)
- results for $\Gamma = \Delta$, $U = 6\Delta$, $\varphi = 0$:

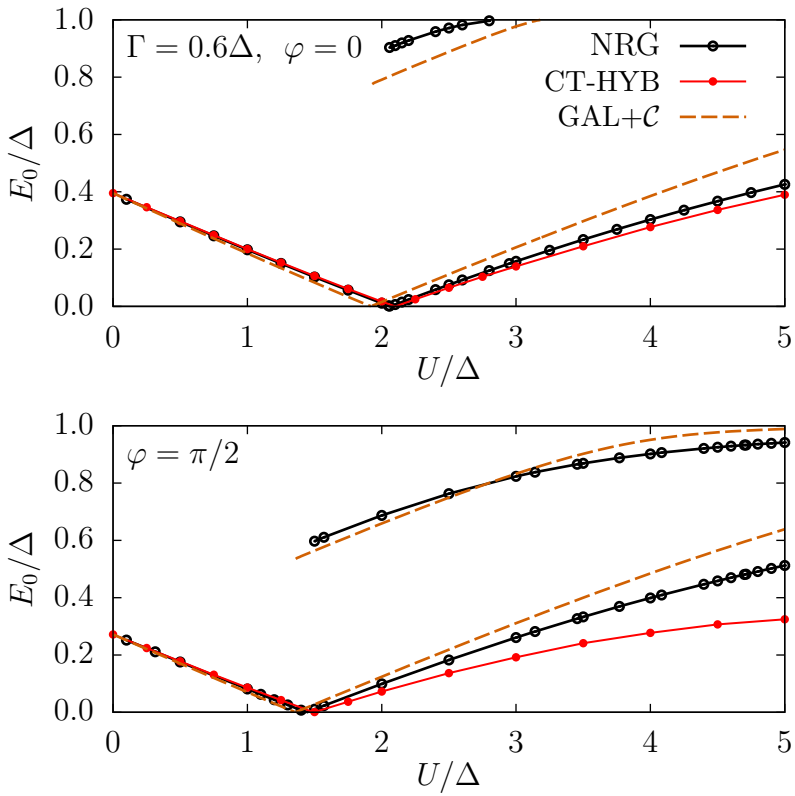


(1) A. Kadlecová, M. Žonda, V. Pokorný, and T. Novotný, Phys. Rev. Applied 11, 044094 (2019).

- low-energy model cannot describe the second pair of ABS in the π (doublet) phase
- how big problem is that?

phase diagram in the $\Gamma - U$ plane:





- $\varphi = 0$: second pair of ABS is bound to low values of Γ and U, far from experimental regime
- $\varphi > 0$: second pair of ABS is always present, but approaches the gap edge

Conclusions

- we introduced two methods to calculate the ABS energies of a superconducting quantum dot system:
- **low-energy model + CT-HYB self-energy:**
  - ✔ reliable method which circumvents the need for analytic continuation of noisy Green function
  - ✔ can be straightforwardly utilized for more complex setups (multi-level dots, multi-dot, multi-terminal setups)
  - ✘ bound to lower values of the interaction strength
  - ✘ does not provide all ABS energies in the π phase
  - ✘ requires high-quality QMC data: computationally expensive
- **generalized atomic limit:**
  - ✔ fast (seconds on a standard PC), simple, provides a reasonable solution in the almost whole parameter space
  - ✔ works well also for double quantum dot systems (1)
  - ✘ problematic away from half-filling without ad-hoc corrections (MGAL)
  - ✘ the correct form of the interaction part not yet known (work in progress)
- both these methods can be used as solvers for superconducting **dynamical mean-field theory**
- GAL can be generalized to **non-equilibrium situations** (e.g., microwave response)

(1) M. Žonda, P. Zalom, T. Novotný, G. Loukeris, J. Bätge, and V. Pokorný, arXiv:2211.10312 (2022).

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