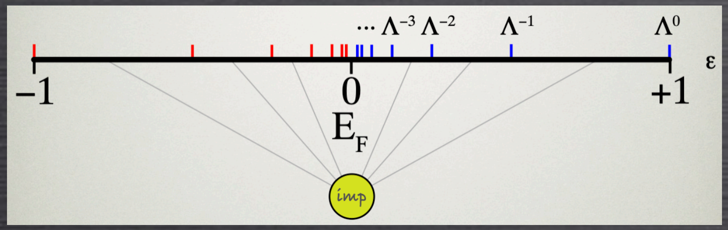
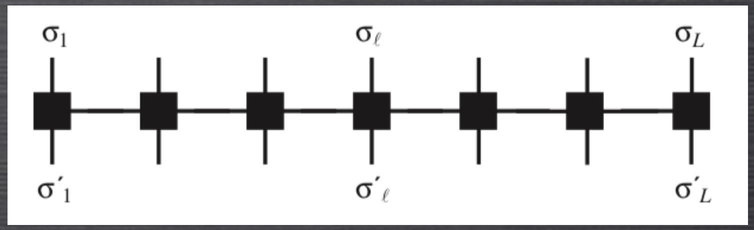
Solvers for quantum impurity problems (with superconducting baths)

Tutorial 5: other methods





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University of Copenhagen, Oct 2021

Zero-bandwidth approximation (ZBW)

Idea: keep only f_0 in the Wilson chain.

Qualitatively describes the nature of the ground state.

Example: Kondo singlet approximated by an AFM state formed between the impurity orbital and the f_0 orbital.

Yu–Shiba–Rusinov screening of spins in double quantum dots

K. Grove-Rasmussen, G. Steffensen, A. Jellinggaard, M. H. Madsen, R. Žitko, J. Paaske & J. Nygård

Nature Communications **9**, Article number: 2376 (2018) | Cite this article

Zero-kinetic-energy approximation

$$H = \sum_{i\sigma} \epsilon_i c^\dagger_{i\sigma} c_{i\sigma} - \alpha d \sum_{i,j} c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} c_{j\downarrow} c_{j\uparrow},$$

$$\epsilon_i \equiv 0$$

$$H = -\frac{g}{L} \sum_{i,j} c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} c_{j\downarrow} c_{j\uparrow} = -\frac{g}{L} \sum_{i,j} A^\dagger_i A_j$$

$$\tilde{H} = H + \tilde{\epsilon} \sum_i \hat{n}_i$$

$$g = 2\alpha$$

$$\tilde{\epsilon} = \alpha d/2 = \alpha/L$$

$$A_j = c_{j\downarrow} c_{j\uparrow}$$

$$[A_i, A^\dagger_j] = \delta_{ij}(1 - \hat{n}_i).$$

$$A_i^2 \equiv 0,$$

$$(A^\dagger_i)^2 \equiv 0,$$

$$A^\dagger_i A_i = P_{2,i} = \hat{n}_{i\uparrow} \hat{n}_{i\downarrow},$$

$$A_i A^\dagger_i = P_{0,i} = 1 - \hat{n}_i + \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

$$P_{\sigma,i} = \hat{n}_{i\sigma}(1 - \hat{n}_{i\bar{\sigma}})$$

$$P_{1,i} = P_{\uparrow,i} + P_{\downarrow,i} = \hat{n}_i - 2\hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

$$B = \frac{1}{\sqrt{U}} \sum_{i}^{U} A_i \qquad \tilde{H} = -hB^\dagger B + \frac{\alpha}{L}\hat{N}$$

$$\tilde{E}_M^{L,U} = -2\alpha \frac{(U-M)M}{L} \qquad \Psi_M = \mathcal{N}_M |M\rangle = \mathcal{N}_M (B^\dagger)^M |0\rangle$$

$$E^{qp,+} = \left(\tilde{E}_{L/2}^{L,L-1} + \tilde{\epsilon}\right) - \mathcal{E} = \left(1 + \frac{1}{L}\right)\alpha.$$

$$E^{qp,-} = \left(\tilde{E}_{L/2-1}^{L,L-1} + \tilde{\epsilon}\right) - \mathcal{E} = \left(1 + \frac{1}{L}\right)\alpha.$$

$$\left(\tilde{E}_{L/2-1}^{L,L-2} + 2\tilde{\epsilon}\right) - \mathcal{E} = 2\alpha$$

L: number of levels.

U: number of unblocked levels.

M: number of Cooper pairs.

$$\bar{v}_i = \langle c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow} c_{i\uparrow} \rangle^{1/2} = \langle A^\dagger_i A_i \rangle^{1/2},$$
$$\bar{u}_i = \langle c_{i\downarrow} c_{i\uparrow} c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} \rangle^{1/2} = \langle A_i A^\dagger_i \rangle^{1/2},$$
$$\bar{\Delta} = \frac{g}{L} \sum_i \bar{v}_i \bar{u}_i,$$
$$\bar{\Delta}' = \frac{g}{L} \sum_i \langle (n_{i\uparrow} n_{i\downarrow} \rangle - \langle n_{i\uparrow} \rangle \langle n_{i\downarrow})\rangle.$$

$$\bar{v}^2 = \frac{M}{U}, \quad \bar{u}^2 = \frac{U-M}{U}, \quad \bar{\Delta} = 2\alpha \frac{\sqrt{M(U-M)}}{U}$$

$$\bar{\Delta}' = \frac{g}{L} \sum_i \langle P_{2,i} \rangle = g \langle P_2 \rangle = 2\alpha \frac{M}{U}.$$

$$H_{\mathrm{QD}} = \frac{J}{L} \sum_{k,k'} \mathbf{S} \cdot \mathbf{s}_{k,k'}$$

$$E_{\mathrm{YSR}} = \left(1 + \frac{1}{L}\right) \alpha - \frac{3J}{4}$$

$$f_\sigma^\dagger \Psi_{L/2}^L = \frac{1}{\sqrt{2}}\frac{1}{\sqrt{L}}\sum_b a_{b,\sigma}^\dagger \Psi_{L/2}^{L\backslash b}$$

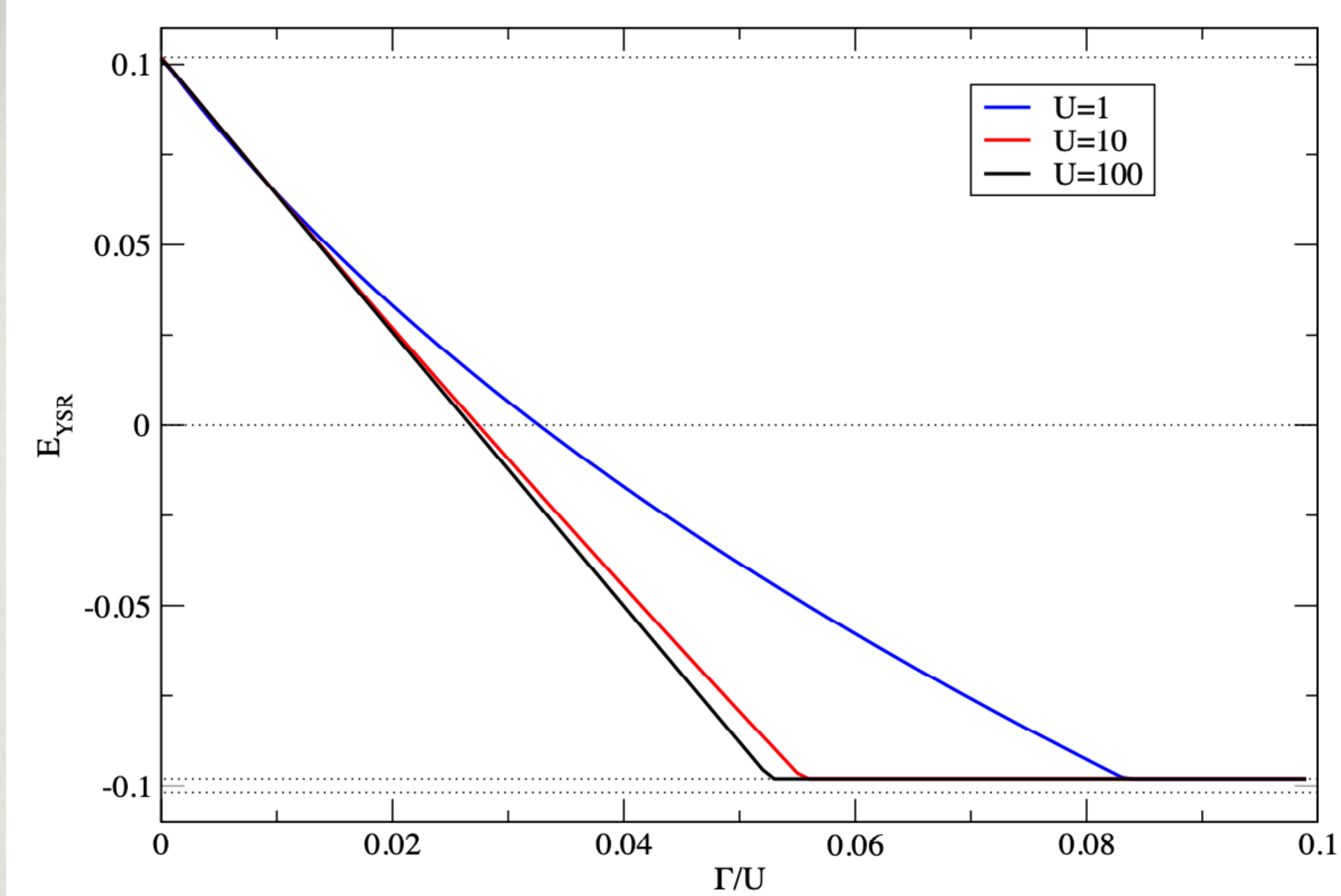
$$f_\uparrow^\dagger f_\downarrow^\dagger \Psi_M^L = \frac{1}{2}\sqrt{\frac{2+L}{L}}\Psi_{M+1}^L + \frac{1}{2}\sqrt{\frac{L-2}{L-1}}\frac{1}{L}\sum_{b\neq b'} a_{b\uparrow}^\dagger a_{b'\downarrow}^\dagger \Psi_M^L$$

$$\begin{aligned}
\psi_0 &= |0\rangle \otimes \Psi_{M+1}^L, \\
\psi_0' &= |0\rangle \otimes a_{b\uparrow}^\dagger a_{b'\downarrow}^\dagger \Psi_M^{L\backslash b,b'} \\
\psi_{1,\sigma} &= |\sigma\rangle \otimes a_{\bar{\sigma}}^\dagger \Psi_M^{L\backslash b} \\
\psi_2 &= |2\rangle \otimes |M\rangle \\
\psi_2' &= |2\rangle \otimes a_{b\uparrow}^\dagger a_{b'\downarrow}^\dagger \Psi_{M-1}^{L\backslash b,b'}
\end{aligned}$$

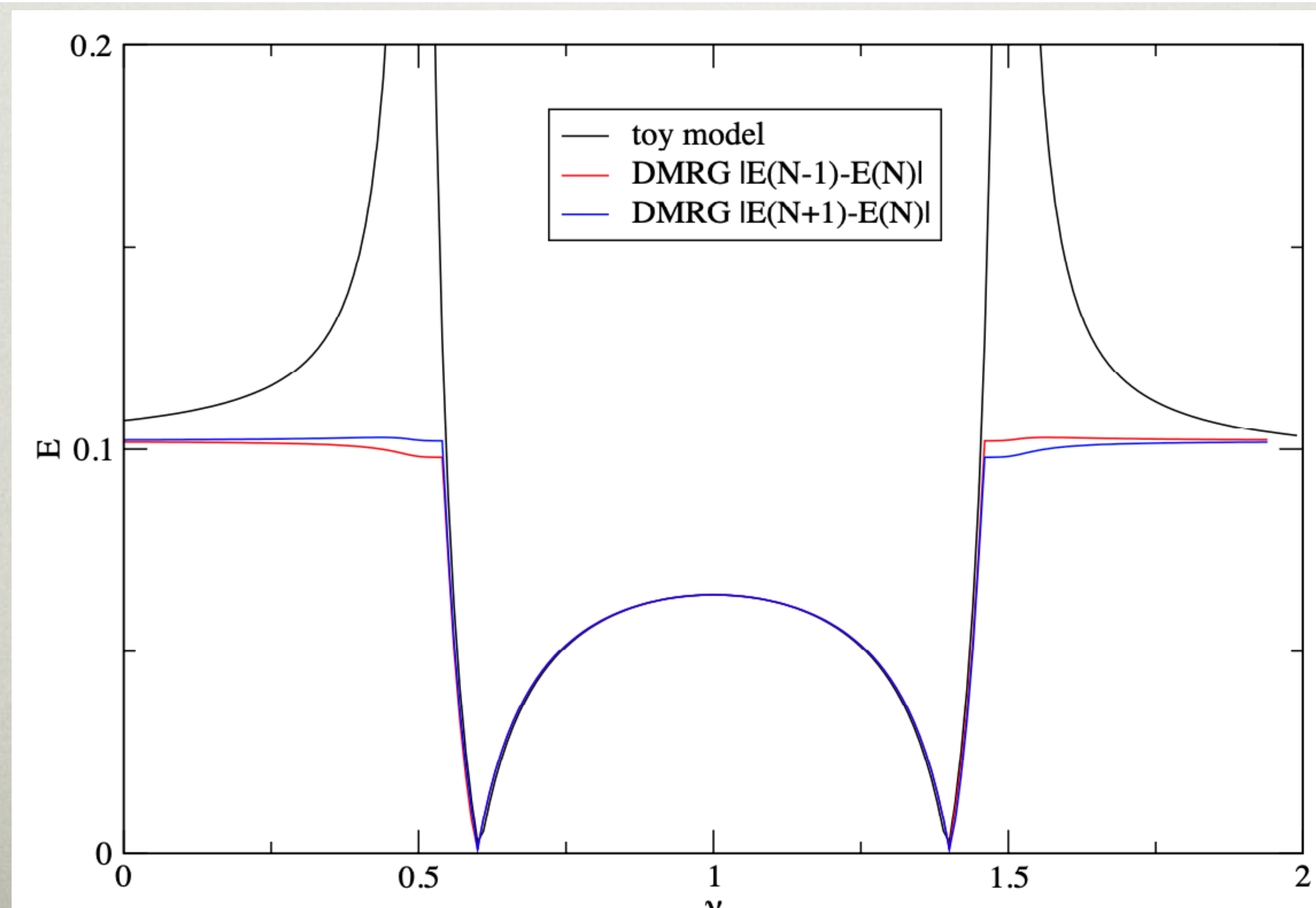
$$\begin{aligned}
\psi_{0,b} &= |0\rangle \otimes |M,b\rangle, \\
\psi_1 &= |1\rangle \otimes |M\rangle, \\
\psi_{2,b} &= |2\rangle \otimes |M-1,b\rangle
\end{aligned}$$

$$H_{\text{eff}} = \begin{pmatrix} E_1^D & v/\sqrt{2} & v/\sqrt{2} \\ v/\sqrt{2} & E_0^D & 0 \\ v/\sqrt{2} & 0 & E_2^D \end{pmatrix}$$

$$H_{\text{eff}} = \begin{pmatrix} E_0^S & 0 & v/2 & v/2 & 0 & 0 \\ 0 & {E^{S'}}_0 & v/2 & v/2 & 0 & 0 \\ v/2 & v/2 & E_1^S & 0 & v/2 & v/2 \\ v/2 & v/2 & 0 & E_1^S & v/2 & v/2 \\ 0 & 0 & v/2 & v/2 & E_2^S & 0 \\ 0 & 0 & v/2 & v/2 & 0 & {E^{S'}}_2 \end{pmatrix}$$

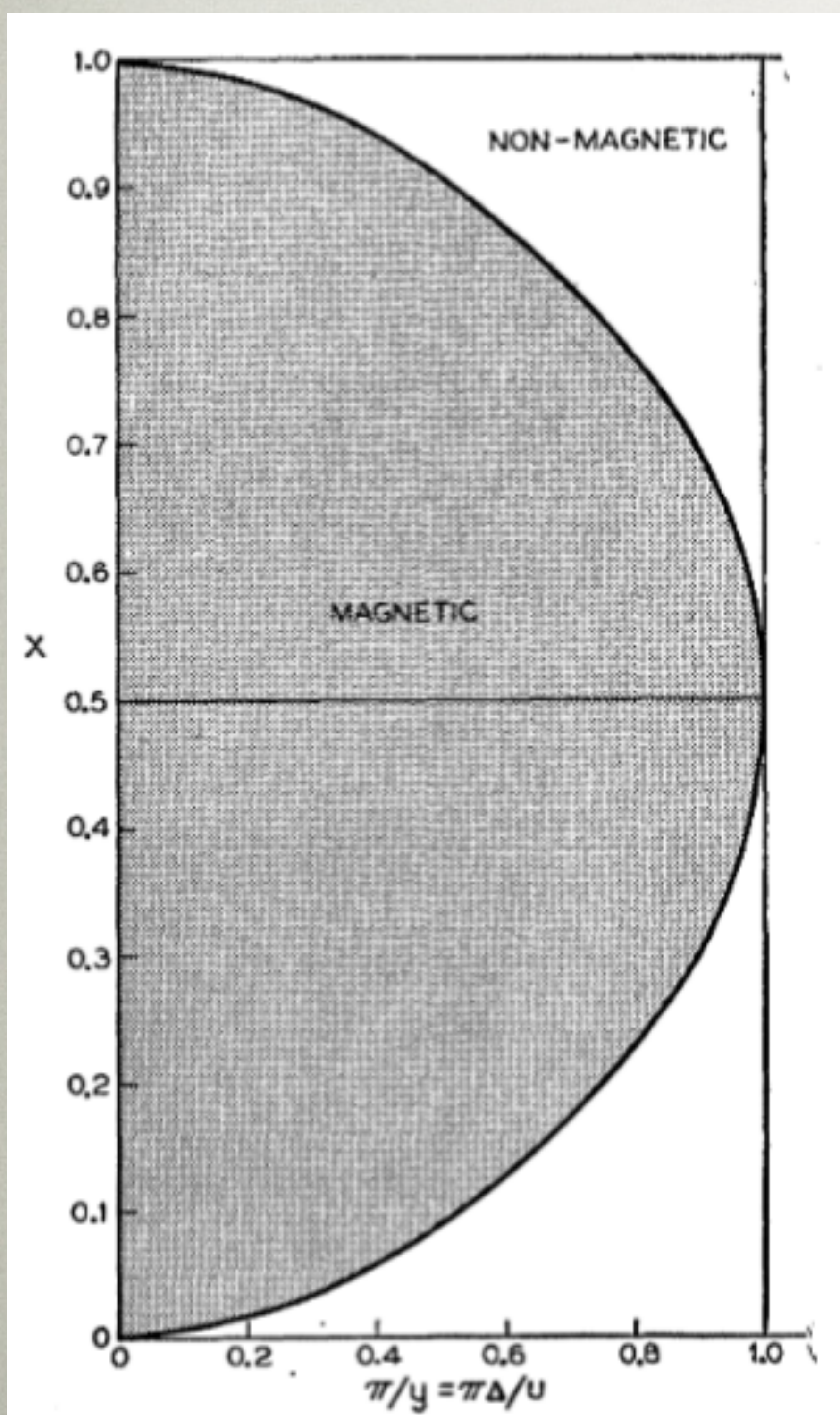


U=1
U=10
U=100
E_{YSR}
Γ/U
0.1
0.05
0
-0.05
-0.1
0
0.02
0.04
0.06
0.08
0.1



toy model
DMRG |E(N-1)-E(N)|
DMRG |E(N+1)-E(N)|
E
0.2
0.1
0
0
0.5
1
1.5
2

Hartree-Fock



$$H = H_0 + H' ,$$

$$H_0 = \sum_{k,\sigma} \varepsilon_k c^{+}_{k\sigma} c_{k\sigma} + \sum_{\sigma} E_d c^{+}_{d\sigma} c_{d\sigma} + V \sum_{k,\sigma} (c^{+}_{k\sigma} c_{d\sigma} + c^{+}_{d\sigma} c_{k\sigma}) - \langle n_d \rangle^2 U ,$$

$$H' = U(c^{+}_{d\uparrow} c_{d\uparrow} - \langle n_d \rangle)(c^{+}_{d\downarrow} c_{d\downarrow} - \langle n_d \rangle) ,$$

$$E_d = \varepsilon_d + \langle n_d \rangle U .$$

requires numerical solution of a transcendent equation

Idea: approximate solution using a single Slater determinant

Anderson 1961
Newns 1969

Perturbation theory (2nd order)

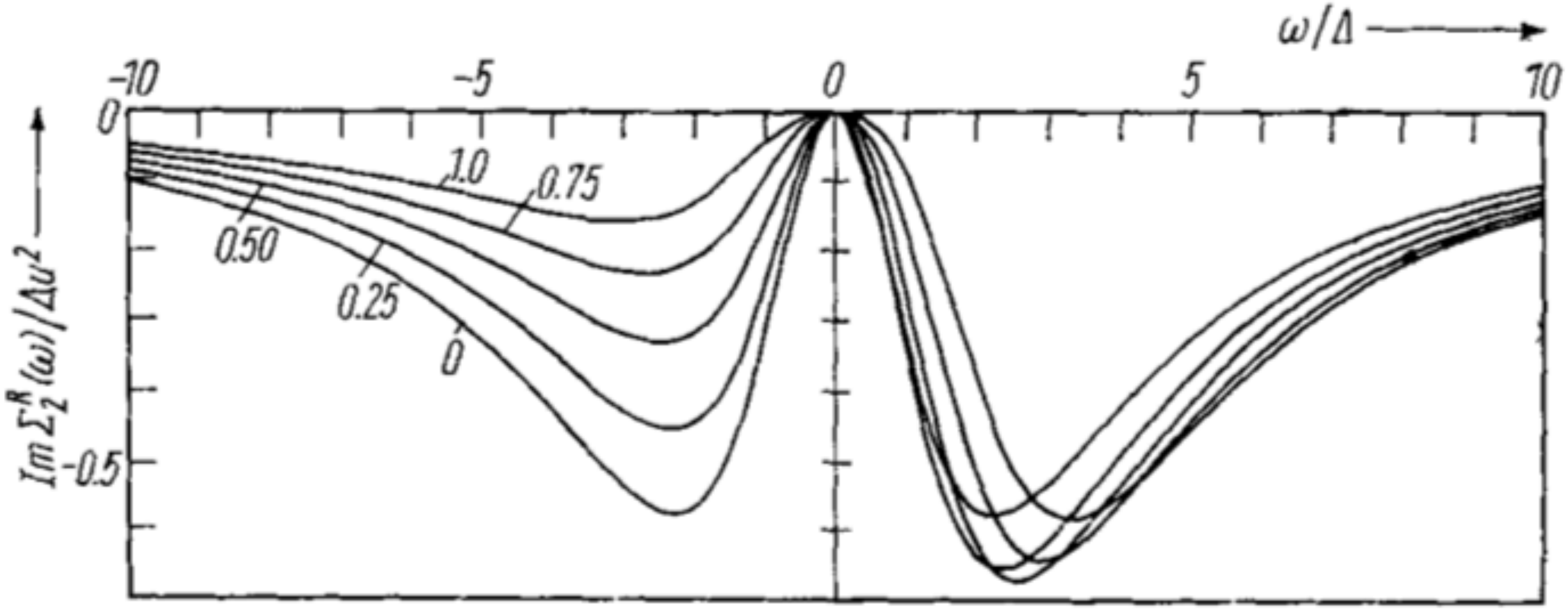
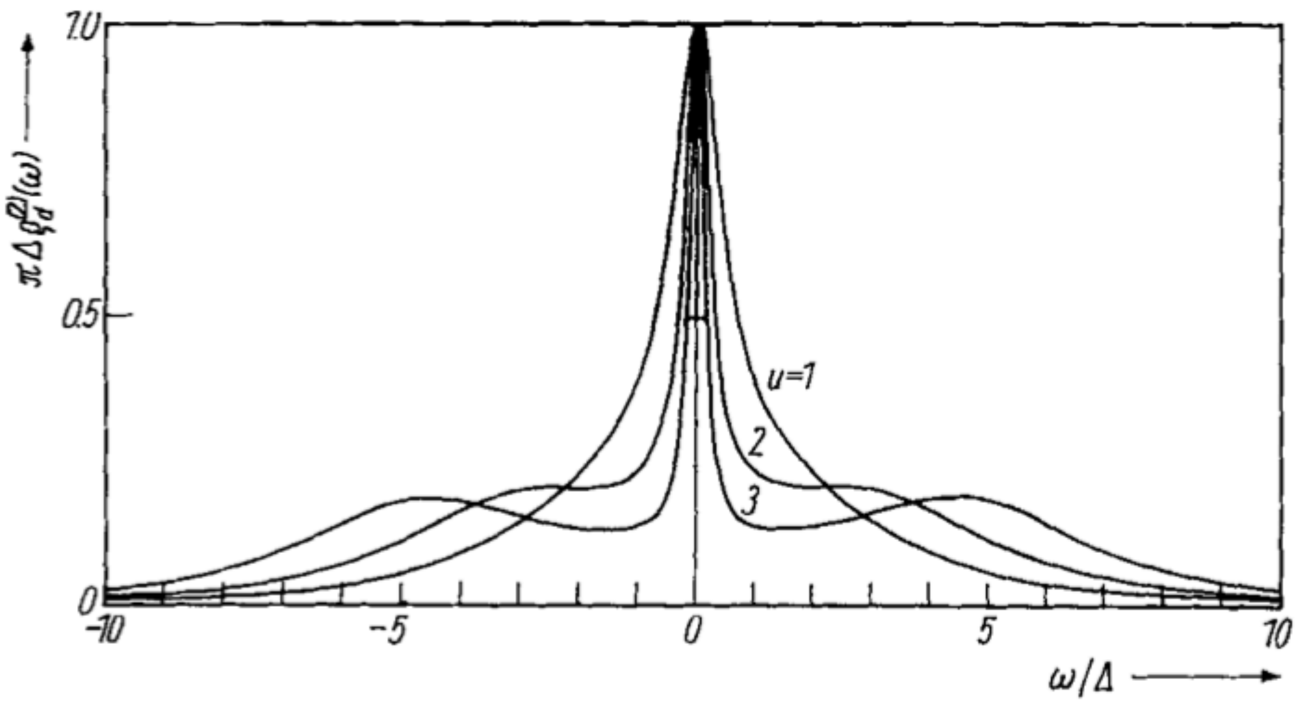


Fig. 2. Imaginary part of $\Sigma_2^{\mathrm{R}}(\omega)$ at $T = 0$ for various values of the asymmetry parameter E_{d}/Δ



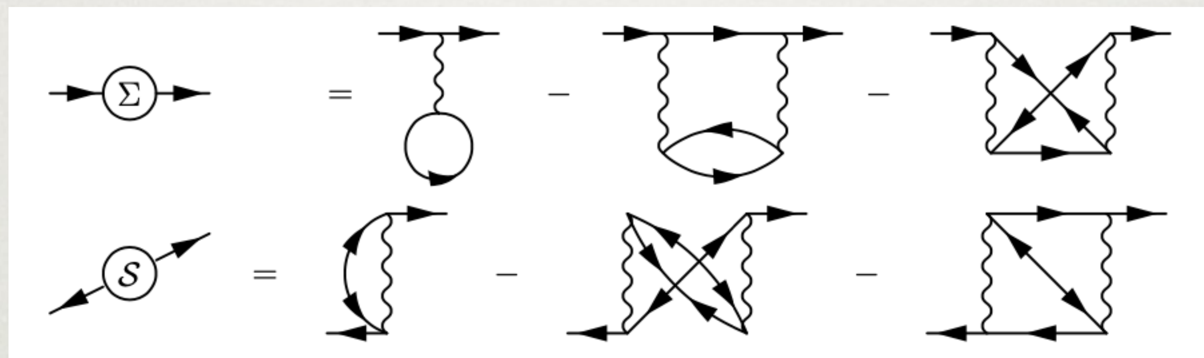
Analytical expressions!

Yosida, Yamada

Horvatić, Zlatić, 1980, 1982

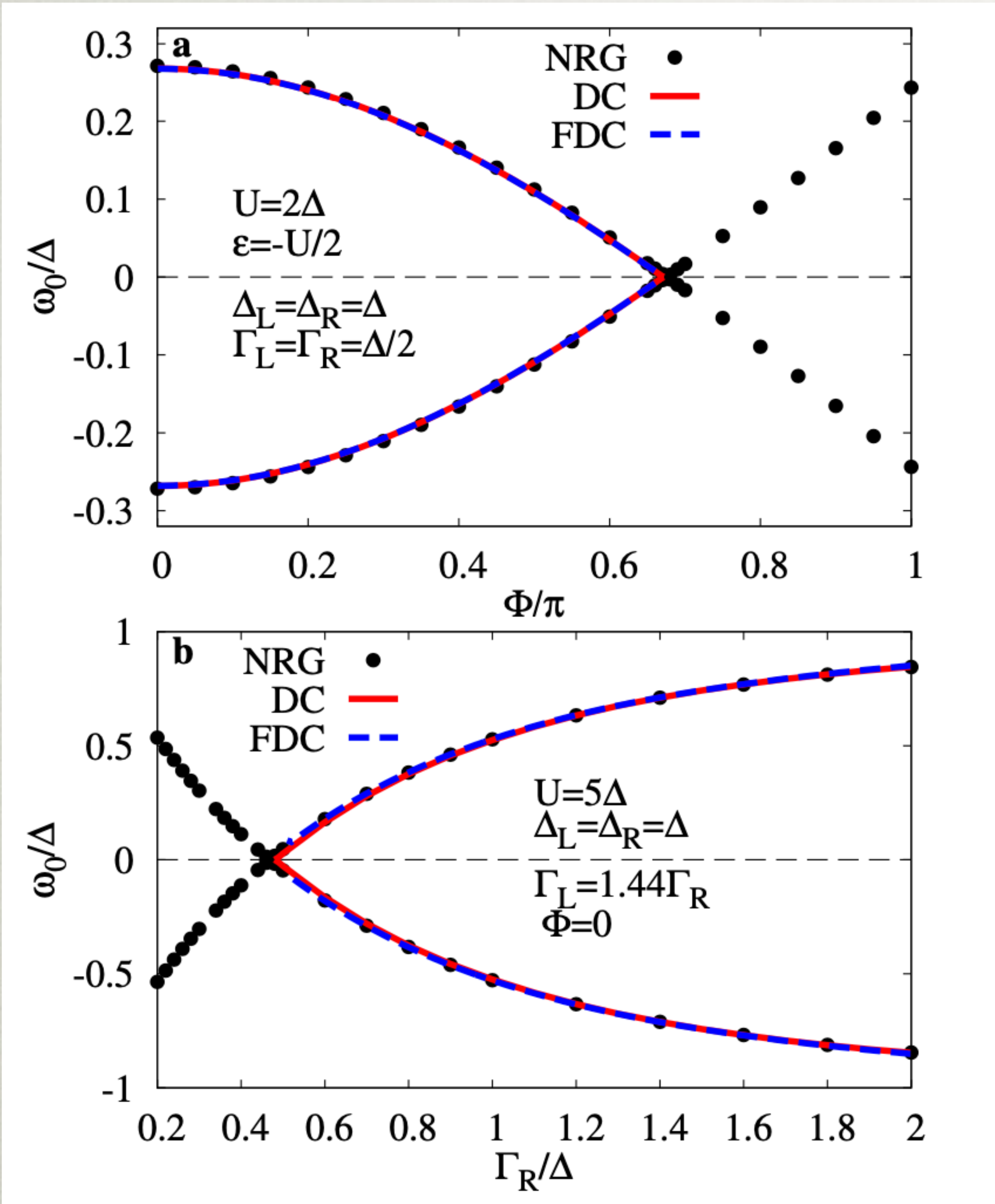
Dynamic corrections (on top of HF)

$$\Sigma^{HF} = \frac{U}{\beta} \sum_{n \in \mathbb{Z}} G(i\omega_n) e^{i\omega_n 0^+} \text{ and } \mathcal{S}^{HF} = \frac{U}{\beta} \sum_{n \in \mathbb{Z}} \mathcal{G}(i\omega_n)$$



$$\Sigma^{(2)}(i\omega_n) = -\frac{U^2}{\beta} \sum_{m \in \mathbb{Z}} G(i\omega_n + i\nu_m)\chi(i\nu_m), \; \mathcal{S}^{(2)}(i\omega_n) = -\frac{U^2}{\beta} \sum_{m \in \mathbb{Z}} \mathcal{G}(i\omega_n + i\nu_m)\chi(i\nu_m).$$

$$\chi(i\nu_m) = \frac{1}{\beta} \sum \left[G(i\omega_n) G(i\omega_n + i\nu_m) + \mathcal{G}(i\omega_n) \mathcal{G}(i\omega_n + i\nu_m) \right]$$



Perturbation theory for an Anderson quantum dot asymmetrically attached to two superconducting leads

M. Žonda, V. Pokorný, V. Janiš, and T. Novotný

Phys. Rev. B **93**, 024523 – Published 29 January 2016

Bethe Ansatz

$$\psi(x_1, x_2, \ldots, x_n) = \sum_{\sigma \in S_n} A(\mathbf{x}, \sigma, \mathbf{p}) g_{p_{\sigma 1}}(x_1) g_{p_{\sigma 2}}(x_2) \cdots g_{p_{\sigma n}}(x_n)$$

$$g_p(x) = \theta(x) e^{ipx + i\delta(p)/2} + \theta(-x) e^{ipx - i\delta(p)/2} \qquad \delta(p) = -2 \arctan\left(\frac{2\Gamma}{p - \epsilon}\right)$$

Problem is integrable if the S matrix satisfies the Yang-Baxter relation.

$$e^{ip_j L + i\delta(p_j)} = \prod_{\alpha=1}^{M} \frac{g(p_j) - \lambda_\alpha + i/2}{g(p_j) - \lambda_\alpha - i/2} \qquad g(p) = \frac{(p - U/2 - \epsilon)^2}{2\Gamma U}$$

$$\prod_{j=1}^{N} \frac{\lambda_\alpha - g(p_j) + i/2}{\lambda_\alpha - g(p_j) - i/2} = -\prod_{\beta=1}^{M} \frac{\lambda_\alpha - \lambda_\beta + i}{\lambda_\alpha - \lambda_\beta - i}$$

BA equations

N. Andrei et al., Rev. Mod. Phys. **55**, 331 (1983)

A. M. Tsvelick, B. Wiegmann, Adv. Phys. **32**, 453 (1983)

Alternative methods (simulations): Quantum Monte Carlo

$$\langle A \rangle = \frac{\mathrm{Tr}\left(Ae^{-\beta H}\right)}{\mathrm{Tr}\left(e^{-\beta H}\right)} \qquad \beta = \frac{1}{k_B T}$$

$$\mathrm{Tr}(e^{-\beta H}) = \mathrm{Tr}\prod_{i=1}^{L} e^{-\Delta\tau H} \qquad \beta = L\Delta\tau$$

imaginary-time discretization

$$e^{-\Delta\tau H} = e^{-\Delta\tau H_1} e^{-\Delta\tau H_2} + \mathcal{O}(\Delta\tau^2)$$

Suzuki-Trotter decomposition

Monte-Carlo sampling over auxiliary variables with Metropolis-Hastings algorithm

Example: Hirsch-Fye QMC algorithm for the Anderson impurity model

Continuous-Time QMC Algorithms

$$H = H_a + H_b$$

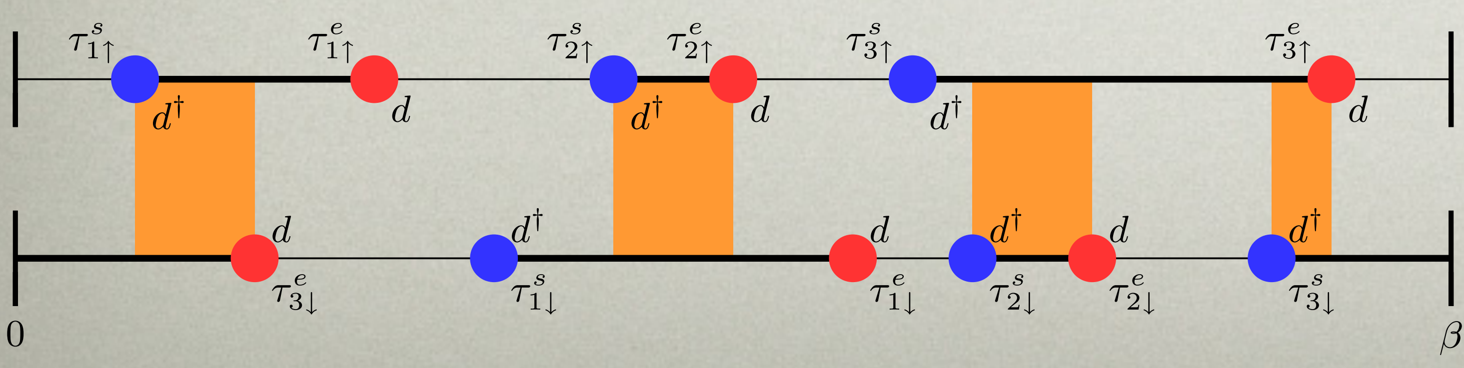
$$\mathrm{Tr}\left(e^{-\beta H}\right) = \mathrm{Tr}\left(T_\tau e^{-\beta H_a} \exp\left[-\int_0^\beta \mathrm{d}\tau\, H_b(\tau)\right]\right)$$

$$= \sum_k \frac{(-1)^k}{k!} \int_0^\beta \mathrm{d}\tau_1 \int_0^\beta \mathrm{d}\tau_2 \cdots \int_0^\beta \mathrm{d}\tau_k \mathrm{Tr}\left(T_\tau e^{-\beta H_a} H_b(\tau_k) H_b(\tau_{k-1}) \cdots H_b(\tau_1)\right)$$

- no time-discretization errors
- no auxiliary-field decomposition

CT-HYB expansion: $H_a = H_{\mathrm{imp}} + H_{\mathrm{band}}$

$$H_b = H_{\mathrm{hyb}}$$



N. V. Prokof'ev et al.,
JETP Lett. **64**, 911 (1996)
P. Werner et al., PRL **97**, 076405 (2006)
K. Haule, PRB **75**, 155113 (2007)
E. Gull et al., RMP **83**, 349 (2011)

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Continuous-time Monte Carlo methods for quantum impurity models

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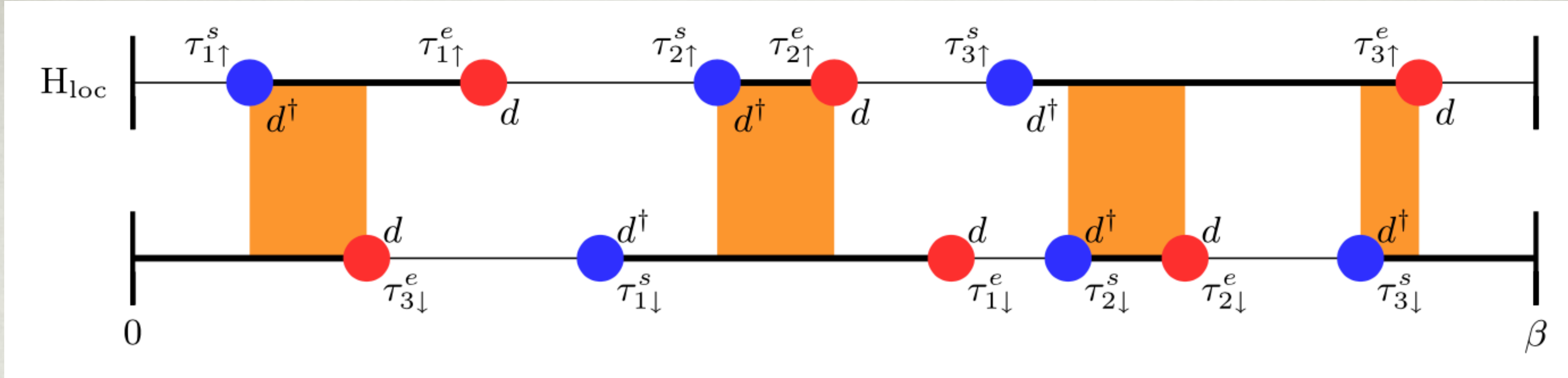
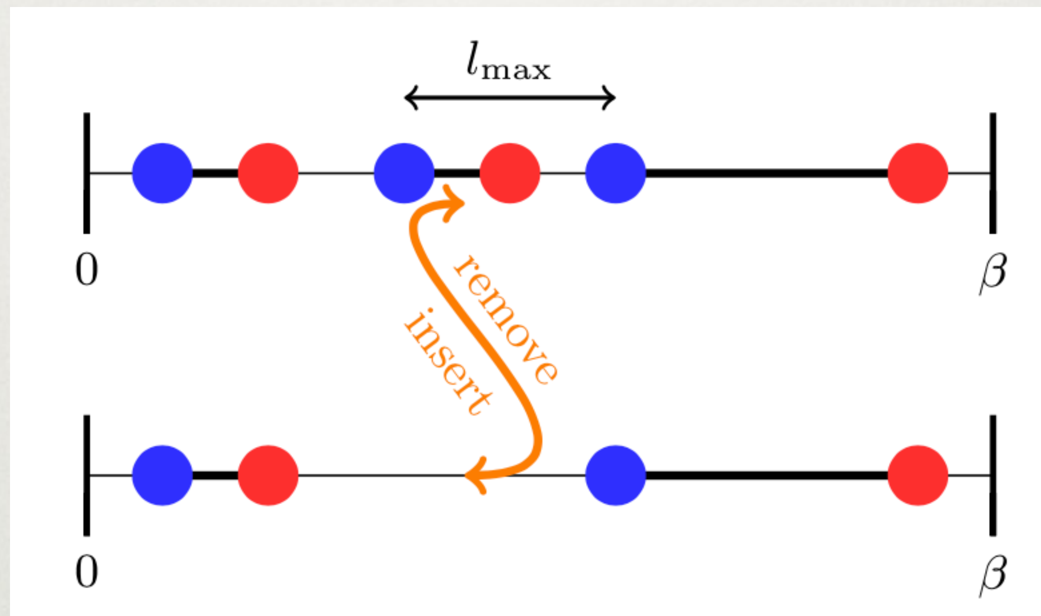
$$H_{\text{hyb}} = \sum_{pj}(V_p^j c_p^\dagger d_j + V_p^{j*} d_j^\dagger c_p) = \tilde{H}_{\text{hyb}} + \tilde{H}_{\text{hyb}}^\dagger$$

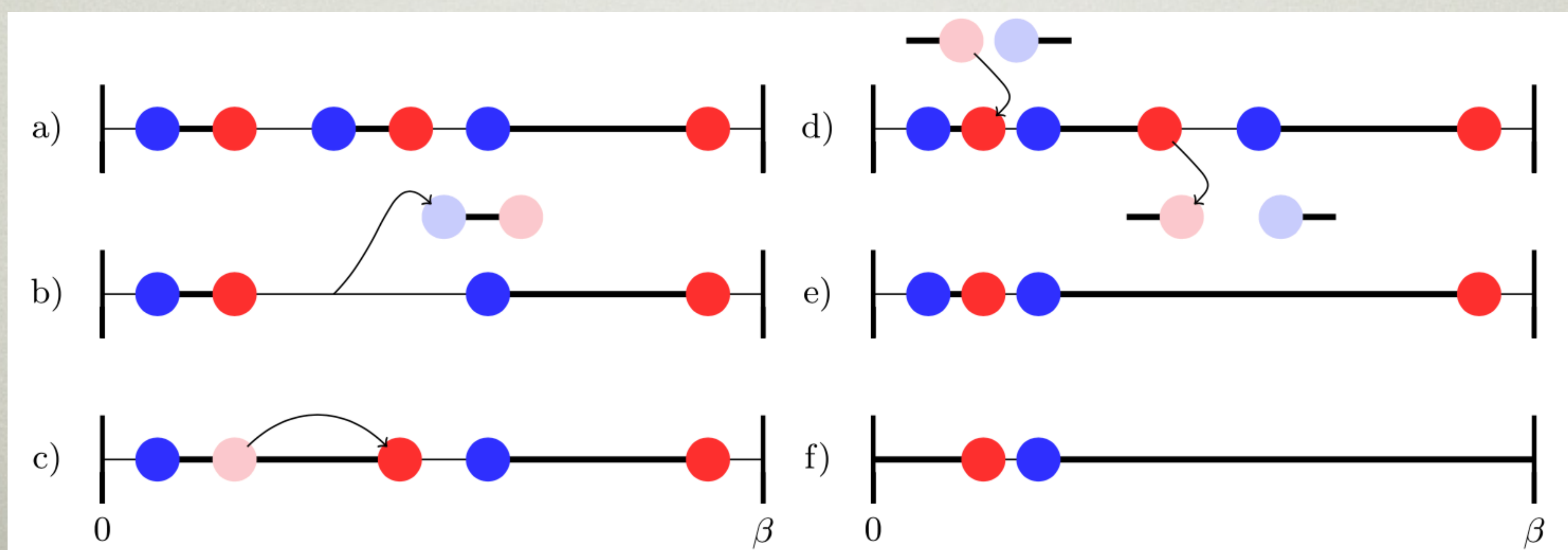
$$Z = \sum_{k=0}^{\infty} \int_0^\beta d\tau_1 \cdots \int_{\tau_{k-1}}^\beta d\tau_k \int_0^\beta d\tau'_1 \cdots \int_{\tau_{k'-1}}^\beta d\tau'_k \times \text{Tr}[T_\tau e^{-\beta H_a} \tilde{H}_{\text{hyb}}(\tau_k) \tilde{H}_{\text{hyb}}^\dagger(\tau'_k) \cdots \times \tilde{H}_{\text{hyb}}(\tau_1) \tilde{H}_{\text{hyb}}^\dagger(\tau'_1)].$$

$$Z = \sum_{k=0}^{\infty} \int_0^\beta d\tau_1 \cdots \int_{\tau_{k-1}}^\beta d\tau_k \int_0^\beta d\tau'_1 \cdots \int_{\tau'_{k-1}}^\beta d\tau'_k \times \sum_{\substack{j_1,\ldots,j_k \\ j'_1,\ldots,j'_k}} \sum_{\substack{p_1,\ldots,p_k \\ p'_1,\ldots,p'_k}} V_{p_1}^{j_1} V_{p'_1}^{j'_1 *} \cdots V_{p_k}^{j_k} V_{p'_k}^{j'_k *} \times \text{Tr}_d[T_\tau e^{-\beta H_{\text{loc}}} d_{j_k}(\tau_k) d_{j'_k}^\dagger(\tau'_k) \cdots d_{j_1}(\tau_1) d_{j'_1}^\dagger(\tau'_1)] \times \text{Tr}_c[T_\tau e^{-\beta H_{\text{bath}}} c_{p_k}^\dagger(\tau_k) c_{p_{k'}}(\tau'_k) \cdots c_{p_1}^\dagger(\tau_1) c_{p'_1}(\tau'_1)].$$

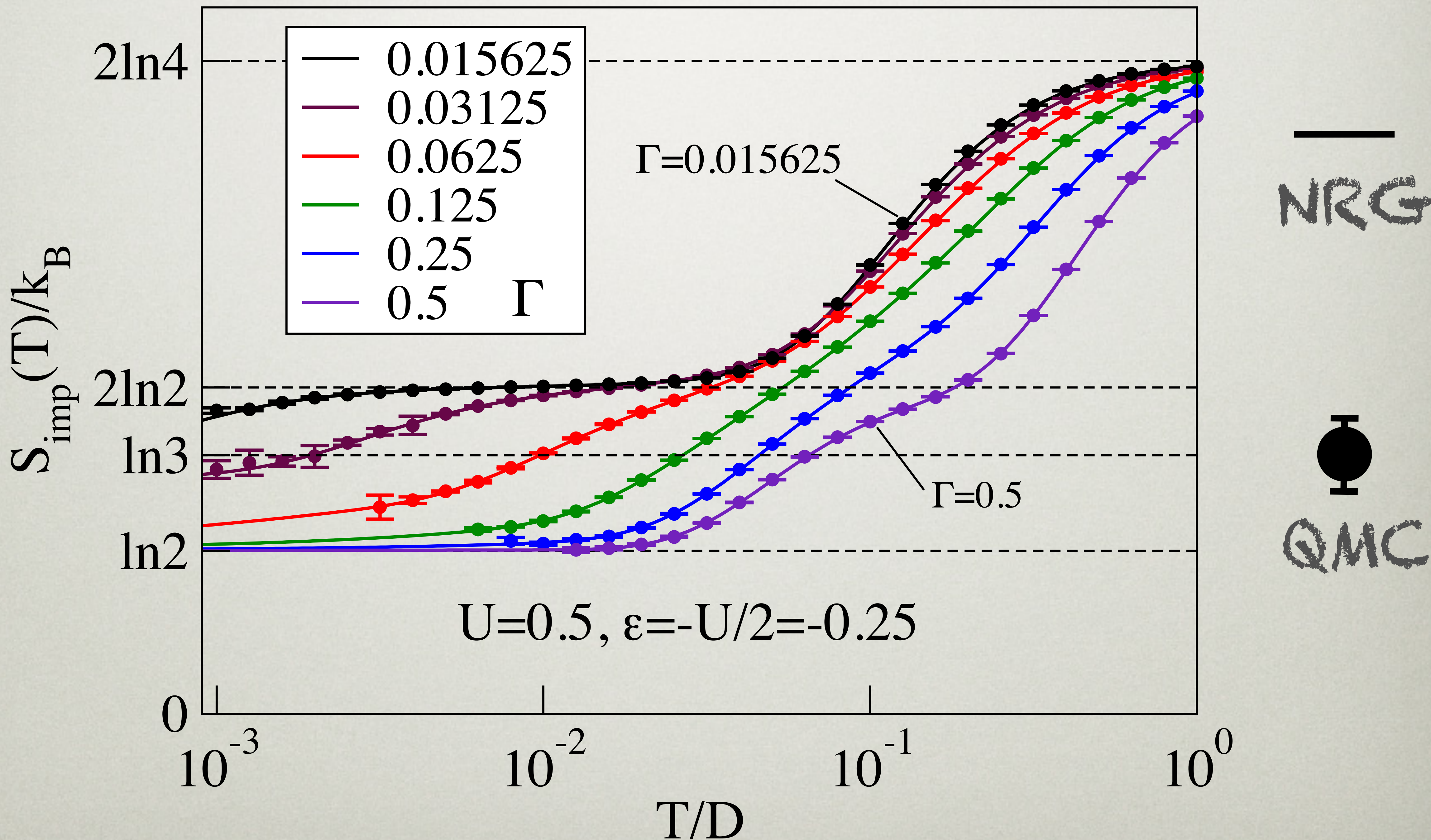
$$Z = Z_{\text{bath}} \sum_k \iiint d\tau_1 \cdots d\tau'_k \sum_{j_1,\ldots,j_k} \sum_{j'_1,\ldots,j'_k} \text{Tr}_d[T_\tau e^{-\beta H_{\text{loc}}} \times d_{j_k}(\tau_k) d_{j'_k}^\dagger(\tau'_k) \cdots d_{j_1}(\tau_1) d_{j'_1}^\dagger(\tau'_1)] \det \mathbf{\Delta}. \quad (9$$


H_{loc}
$\tau^s_{1\uparrow}$ $\tau^e_{1\uparrow}$ $\tau^s_{2\uparrow}$ $\tau^e_{2\uparrow}$ $\tau^s_{3\uparrow}$ $\tau^e_{3\uparrow}$
$d^\dagger$ d $d^\dagger$ d $d^\dagger$ d
d $d^\dagger$ d $d^\dagger$ d $d^\dagger$
$\tau^e_{3\downarrow}$ $\tau^s_{1\downarrow}$ $\tau^e_{1\downarrow}$ $\tau^s_{2\downarrow}$ $\tau^e_{2\downarrow}$ $\tau^s_{3\downarrow}$
0
β


$l_{\max}$
0
β
remove
insert
0
β

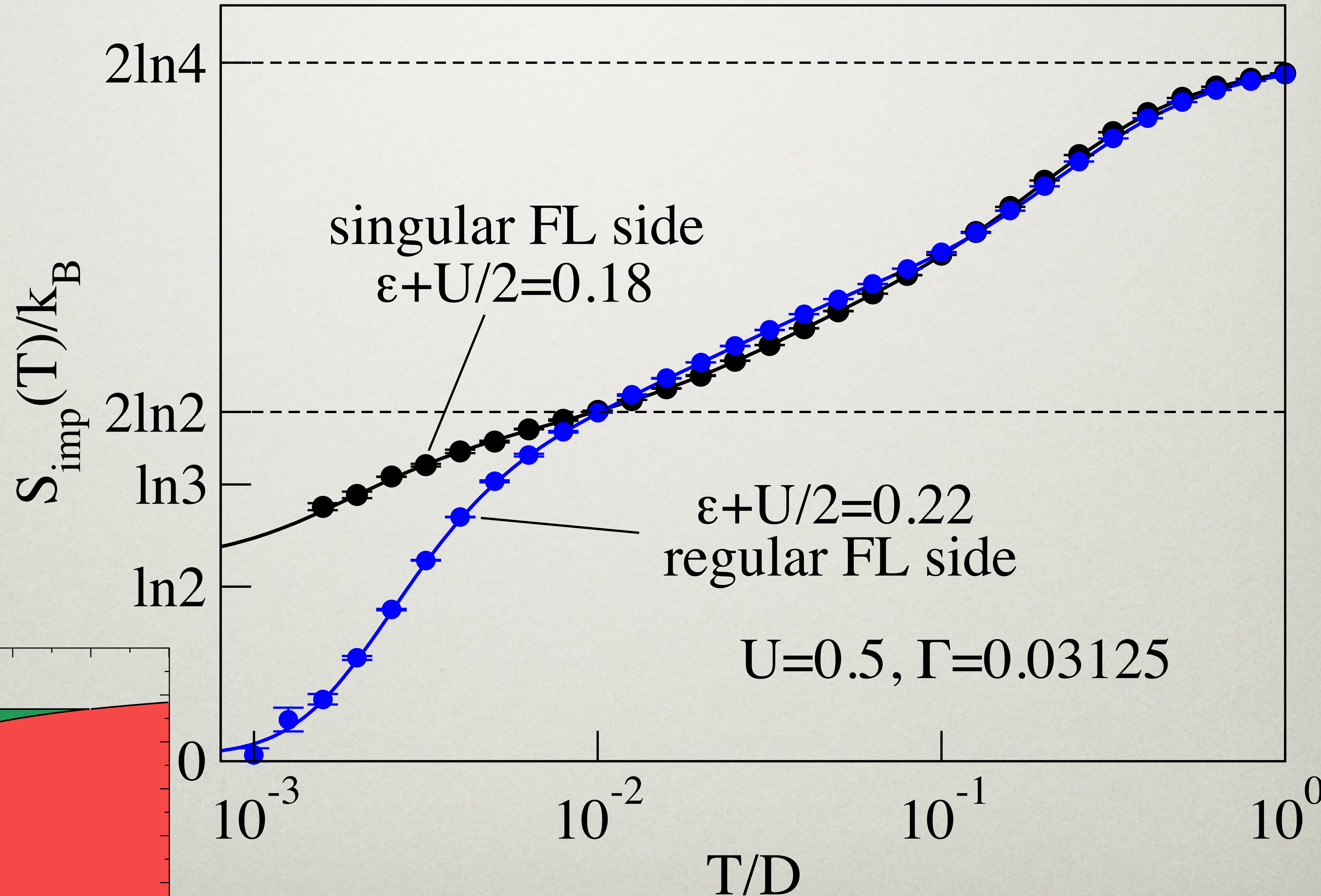

a)
b)
c)
d)
e)
f)
0
β
0
β

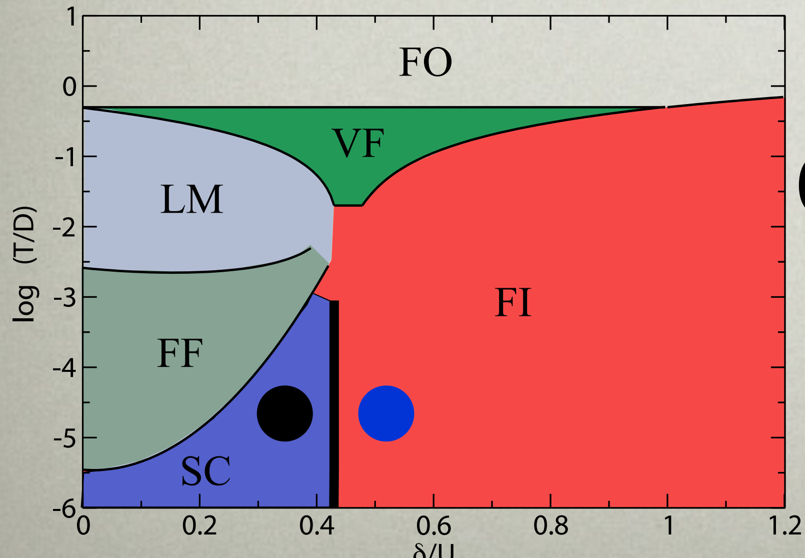
Do NRG and QMC agree?



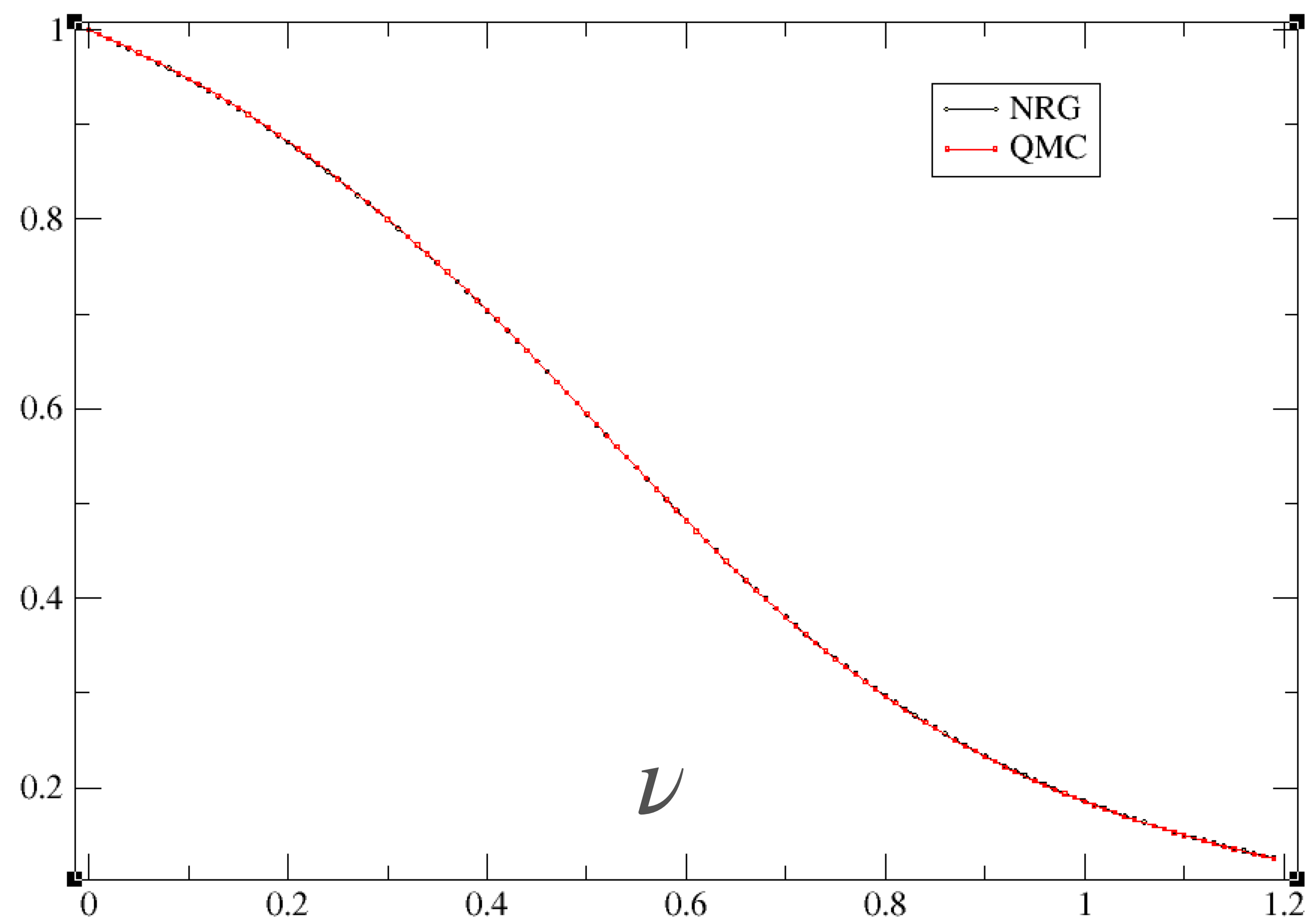
R. Žitko, J. Mravlje, K. Haule, Phys. Rev. Lett. **108**, 066602 (2012)

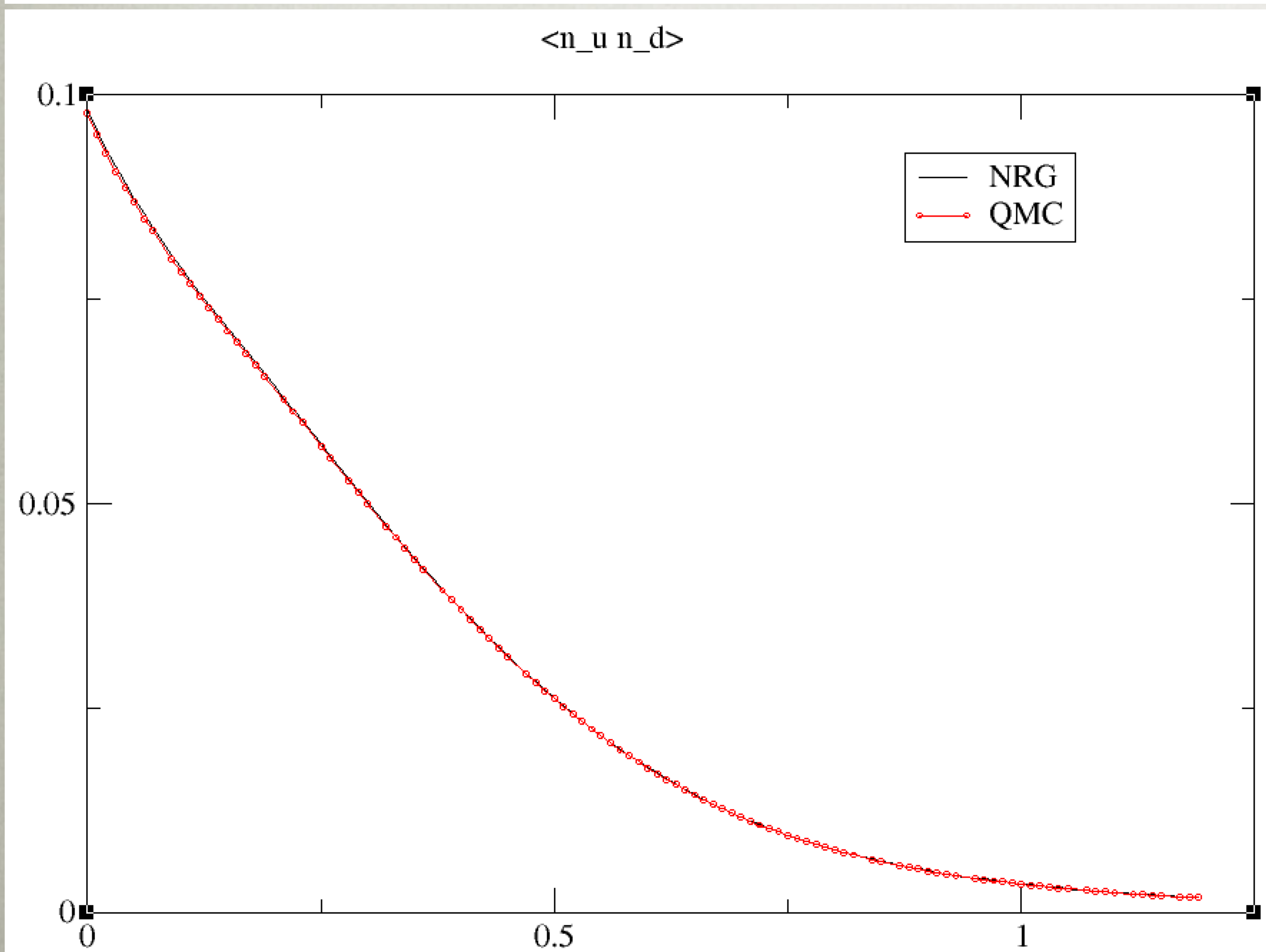
Evidence for a Quantum Phase Transition





R. Žitko, J. Mravlje, K. Haule, Phys. Rev. Lett. **108**, 066602 (2012)





$\beta = 350$

NRG, FDM algorithm

$\Lambda = 1.8$

U=1.2, $\Gamma = 0.2, \Delta = 0.05$

NON-CROSSING APPROXIMATION

$$d_\sigma = b^\dagger f_\sigma$$

$$H_{\rm SB} = \sum_{k_L,\sigma} \varepsilon_{k_L,\sigma}\, a^\dagger_{k_L\sigma} a_{k_L\sigma} + \sum_{k_L} \Delta(a^\dagger_{k_L\uparrow} a^\dagger_{-k_L\downarrow} + h.c.) + \sum_\sigma \varepsilon_\sigma f^\dagger_\sigma f_\sigma + \frac{\overline{V}_L}{\sqrt{N}} \sum_{k_L,\sigma} \left(c^\dagger_{k_L,\sigma} b^\dagger f_\sigma + h.c.\right) + (L \to R)$$
$$+ \lambda\left(\sum_\sigma f^\dagger_\sigma f_\sigma + b^\dagger b - 1\right).$$

Zero-Bias Anomaly in a Nanowire Quantum Dot Coupled to Superconductors

Eduardo J. H. Lee, Xiaocheng Jiang, Ramón Aguado, Georgios Katsaros, Charles M. Lieber, and Silvano De Franceschi
Phys. Rev. Lett. **109**, 186802 – Published 31 October 2012