Some new analytical and numerical approaches to an SU(N) impurity Anderson model

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Collaboration in related works: Tatsuya Fujii[2]

Outline

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(3) Green's function in high-energy solvable limits: $T \to \infty$ and $eV \to \infty$,

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(4) Low-energy properties: 1/(N -1) expansion based on a perturbation in U

Zero order in 1/(N -1) : Hartree-Fock (HF)
Leading order in 1/(N -1) : HF-RPA
Higher order terms : *Fluctuations beyond HF-RPA*

(5) Green's function at low temperatures: order $1/(N-1)^2$ and NRG results:

- *Renormalization factor Z, Wilson ratio R, …. , away from half-filling*
- *Green's function G(ω) in the electron-hole symmetric case*

(6) Summary

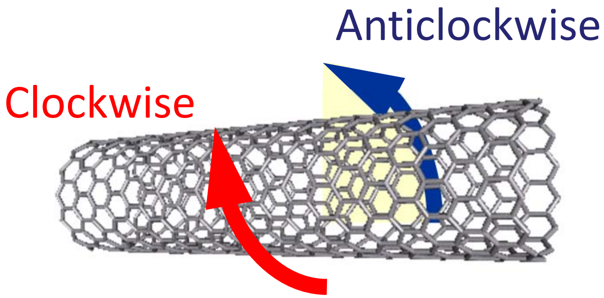
R. Sakano, T. Fujii, & A.O, PRB 83 (2011),
A.O, R. Sakano, & T. Fujii, PRB 84 (2011),
A.O, PRB 85 (2012),
A.O and R. Sakano, PRB 91 (2015),
A.O, M. Awane, & R. Sakano.

Introduction

Main interest: *Kondo effect in quantum dots*

Orbital degeneracy gives a variety to the Kondo physics:

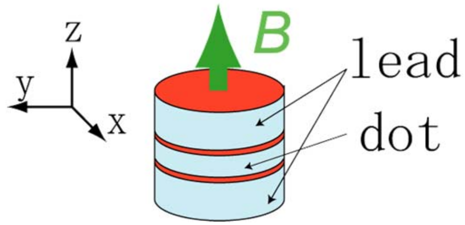
- Carbon nanotube dot

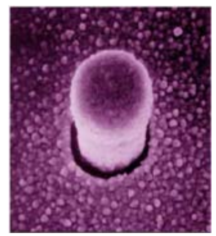


T. Delattre, *et al*., Nat. Phys. (2009)

M. Ferrier, T. Arakawa, …, & K. Kobayashi

- Vertical quantum dot



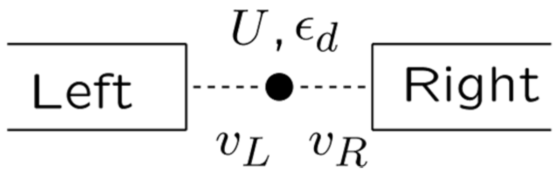


S. Tarucha, *et al.*, PRL (1996)

SU(N) Anderson model describes the essential physics of orbital Kondo systems:

We study Green's function over a wide energy scales using several different approaches:
1/(N-1) expansion, Numerical renormalization group (NRG),
Non-crossing approximation (NCA), and also an exact result in $eV \to \infty$

N-fold degenerate Anderson model:

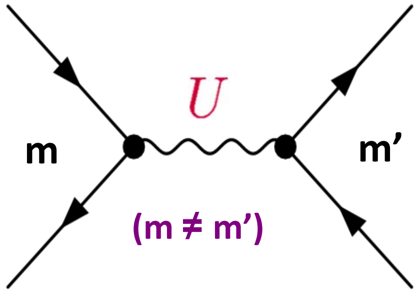


$$\mathcal{H} = \mathcal{H}_d + \mathcal{H}_T + \mathcal{H}_c \,,$$

$$\mathcal{H}_d = \sum_{m=1}^{N} \epsilon_d \, n_{dm} + \frac{U}{2} \sum_{\substack{m,m' \\ (m \neq m')}} n_{dm} \, n_{dm'} \,,$$

$$\mathcal{H}_c = \sum_{\alpha=L,R} \sum_{m=1}^{N} \int_{-D}^{D} d\epsilon \, \epsilon \, c^{\dagger}_{\epsilon\alpha m} c_{\epsilon\alpha m} \,,$$

$$\mathcal{H}_T = \sum_{\alpha=L,R} \sum_{m=1}^{N} v_{\alpha} \left(d^{\dagger}_{m} \, \psi_{\alpha m} + \text{H.c.} \right) ,$$



$$n_{dm} \equiv d^{\dagger}_{m} d_{m}$$

Level width: $\Delta \equiv \Gamma_L + \Gamma_R$

$$\Gamma_{\alpha} \equiv \pi \rho \, v_{\alpha}^{2} \,, \qquad \rho = \frac{1}{2D}$$

$$\psi_{\alpha m} \equiv \int_{-D}^{D} d\epsilon \, \sqrt{\rho} \, c_{\epsilon\alpha m}$$

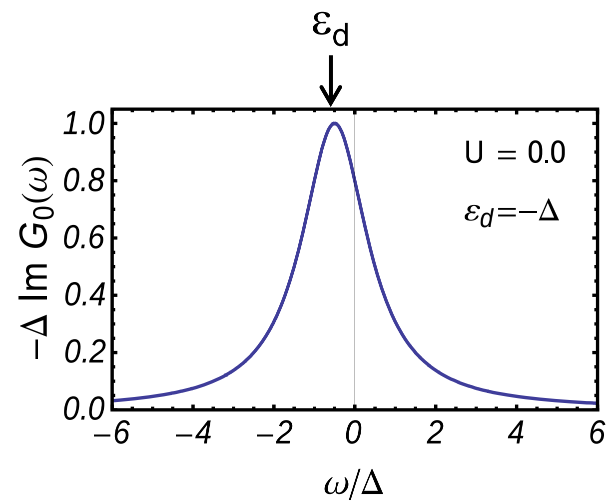
- Conduction band also has N-fold degeneracy
- Hybridization *preserves the orbital index "m"*
- This system has an SU(N) symmetry, which for N=2 describes the *spin degeneracy*.

Two possible starting points

- Non-interacting limit: $U = 0$

Green's function: $$G_m^0(\omega) = \frac{1}{\omega - \epsilon_d + i\Delta}$$

Impurity level becomes a resonance of the width $\Delta = \pi\rho v^2$ at $\omega = \varepsilon_d$



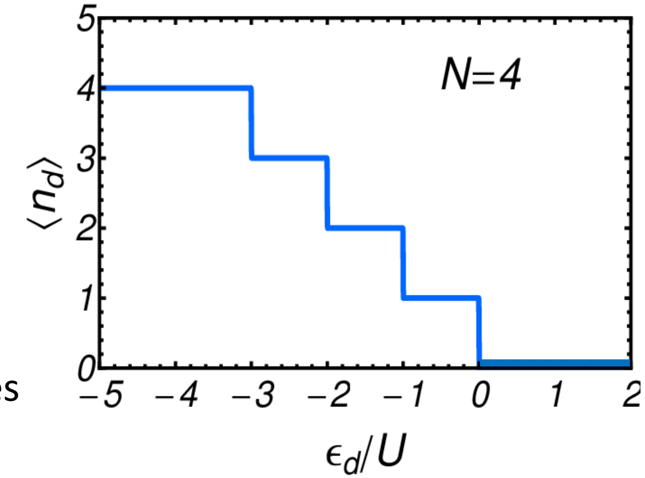
- Atomic limit: $\Delta = 0$

$$\mathcal{H}_d = \sum_{m=1}^{N} \epsilon_d n_{dm} + \frac{U}{2} \sum_{\substack{m,m' \\ (m\neq m')}} n_{dm'} n_{dm}$$

Eigenvalue: $$E_Q = \epsilon_d Q + \frac{U}{2} Q(Q-1), \qquad 0 \le Q \le N$$

Impurity occupation $\langle n_{dm} \rangle$ discontinuously changes as ε_d varies at $\varepsilon_d = 0, -U, -2U, \cdots, -(N-1)U$.

Coulomb Oscillation (period U)



Green's function at $T \rightarrow \infty$, and $eV \rightarrow \infty$

Atomic limit, *NCA*, and *exact results*

$$G_m(\omega) = \int_0^\infty dt \, \langle d_m(t) \, d_m^\dagger(0) \rangle \, e^{i(\omega + i\delta)t}$$

Atomic limit Green's function

Partition function: $\Xi = \sum_{\mathcal{Q}=0}^{N} \binom{N}{\mathcal{Q}} e^{-\beta E_{\mathcal{Q}}}, \qquad E_{\mathcal{Q}} = \mathcal{Q}\,\epsilon_d + \frac{U}{2}\mathcal{Q}\,(\mathcal{Q}-1)$

Green's function: $G_m^{\mathrm{ATM}}(\omega) = \frac{1}{\Xi} \sum_{\mathcal{Q}=0}^{N-1} \binom{N-1}{\mathcal{Q}} \frac{e^{-\beta E_{\mathcal{Q}+1}} + e^{-\beta E_{\mathcal{Q}}}}{\omega - \left(E_{\mathcal{Q}+1} - E_{\mathcal{Q}}\right)}$

- In the limit of $T \to \infty$;

$$G_m^{\mathrm{ATM}}(\omega) \xrightarrow{T\to\infty} \frac{1}{2^{N-1}} \sum_{\mathcal{Q}=0}^{N-1} \binom{N-1}{\mathcal{Q}} \frac{1}{\omega - \underbrace{\left(E_{\mathcal{Q}+1} - E_{\mathcal{Q}}\right)}_{\epsilon_{d,m} + U\mathcal{Q}}};$$

This can be generalized to m-dependent level $\epsilon_{d,m}$ in a finite magnetic field

Continued Fraction form:

$$G_m^{\mathrm{ATM}}(\omega) \to \cfrac{1}{\omega - \xi_{d,m} - \cfrac{\mathcal{B}_1 \left(\frac{U}{2}\right)^2}{\omega - \xi_{d,m} - \cfrac{\mathcal{B}_2 \left(\frac{U}{2}\right)^2}{\ddots - \cfrac{\ddots}{\omega - \xi_{d,m} - \cfrac{\mathcal{B}_{N-1}\left(\frac{U}{2}\right)^2}{\omega - \xi_{d,m}}}}}}$$

$$\xi_{d,m} = \epsilon_{d,m} + \frac{(N-1)U}{2},$$

$$\mathcal{B}_k = k\,(N-k),$$

Exact equilibrium finite-U NCA Green's function in $T \to \infty$ limit

- At $T \to \infty$; $\qquad G_m^{\mathrm{NCA}}(\omega) = G_m^{\mathrm{ATM}}(\omega + iN\Delta),$

Partial Fraction form:

$$G_m^{\mathrm{NCA}}(\omega) \xrightarrow{T\to\infty} \frac{1}{2^{N-1}} \sum_{Q=0}^{N-1} \binom{N-1}{Q} \frac{1}{\omega - \xi_{d,m} + i\,N\Delta}; \qquad \xi_{d,m} = \epsilon_{d,m} + \frac{(N-1)U}{2},$$

Continued Fraction form:

$$G_m^{\mathrm{NCA}}(\omega) \to \cfrac{1}{\omega - \xi_{d,m} + i\,N\Delta - \cfrac{\mathcal{B}_1\left(\frac{U}{2}\right)^2}{\omega - \xi_{d,m} + i\,N\Delta - \cfrac{\mathcal{B}_2\left(\frac{U}{2}\right)^2}{\ddots - \cfrac{\ddots}{\omega - \xi_{d,m} + i\,N\Delta - \cfrac{\mathcal{B}_{N-1}\left(\frac{U}{2}\right)^2}{\omega - \xi_{d,m} + i\,N\Delta}}}}}$$

$$\mathcal{B}_k = k\,(N-k)\,,$$

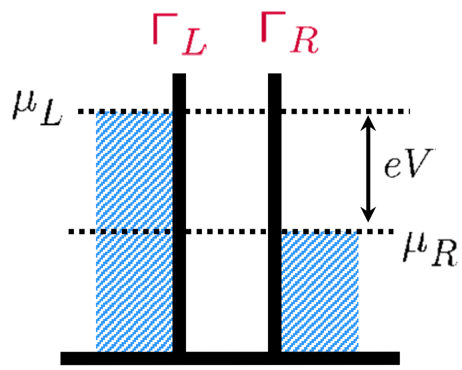
A.O and R. Sakano, A.O, PRB 91 (2015)

Exact Green's function at high-energy scale

- High-bias limit $eV \to \infty$, *or* High-temperature limit $T \to \infty$:

*The exact result discribes the relaxation processes at high energies, determined by **one incident particle + k-1 particle-hole pairs** (k=1,2,…,N-1)*

2k-1 Fermions



$$G^r_m(\omega) = \cfrac{1}{\omega - \xi_{d,m} - \mathcal{A}_1 \frac{rU}{2} + i\Delta - \cfrac{\mathcal{B}_1 (1-r^2)\left(\frac{U}{2}\right)^2}{\omega - \xi_{d,m} - \mathcal{A}_2 \frac{rU}{2} + i\,3\Delta - \cfrac{\mathcal{B}_2 (1-r^2)\left(\frac{U}{2}\right)^2}{\ddots - \cfrac{\ddots}{\omega - \xi_{d,m} - \mathcal{A}_{N-1}\frac{rU}{2} + i\,(2N-3)\Delta - \cfrac{\mathcal{B}_{N-1}(1-r^2)\left(\frac{U}{2}\right)^2}{\omega - \xi_{d,m} - \mathcal{A}_N \frac{rU}{2} + i\,(2N-1)\Delta}}}}}$$

Coefficients: $\mathcal{A}_k = N - 1 - 2(k-1), \quad \mathcal{B}_k = k\,(N-k), \quad \mathcal{C}_k = 2k-1.$

Hybridization asymmetry: $r \equiv \dfrac{\Gamma_L - \Gamma_R}{\Gamma_L + \Gamma_R}.$

(***r*** *varies impurity occupation from* 1/2)

*For r =0, this expression also describes the exact **equilibrium Green's function** at T→ ∞*

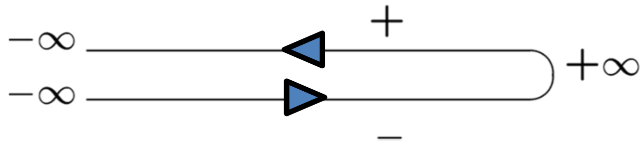
This result can be used for testing approximate methods in high-energy limit

The analytic solution has been obtained using an effective non-Hermitian Hamiltonian defined with respect to a Liouville-Fock space, or a thermal field theory.

A.O and R. Sakano, PRB 91 (2015), PRB 88 (2013)

R.B.Saptsov & M.R.Wegewijs, PRB 86 (2012)
[related work for *N*=2 at *T*→∞]

Time evolution along Keldysh contour



Effective action: $$Z_{\rm eff} = \int D\bar{\eta}\, D\eta\ e^{i\,(S_0+S_U)}\ ,\qquad \boldsymbol{\eta}_m = \begin{bmatrix} \eta_{m-} \\ \eta_{m+} \end{bmatrix}$$

$$S_U = -\sum_{m>m'} U \int_{-\infty}^{\infty} dt \left[\, \overline{\eta}_{m-}(t)\, \eta_{m-}(t)\, \overline{\eta}_{m'-}(t)\, \eta_{m'-}(t) \ -\ \overline{\eta}_{m+}(t)\, \eta_{m+}(t)\, \overline{\eta}_{m'+}(t)\, \eta_{m'+}(t) \,\right]$$

$eV \to \infty$

$$S_0 = \sum_{m=1}^{N} \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dt'\ \overline{\boldsymbol{\eta}}_m(t)\, \boldsymbol{K}_{0,m}(t,t')\, \boldsymbol{\eta}_m(t') \ \Longrightarrow\ \sum_{m=1}^{N} \int_{-\infty}^{\infty} dt\ \overline{\boldsymbol{\eta}}_m(t)\, \boldsymbol{\tau}_3 \left\{ \mathbf{1}\left(i\frac{\partial}{\partial t} - \epsilon_{d,m}\right) - \boldsymbol{L}_0 \right\} \boldsymbol{\eta}_m(t)$$

$$\boldsymbol{K}_{0,m}(t,t') = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \left\{ \boldsymbol{G}_{0,m}(\omega) \right\}^{-1} e^{-i\omega(t-t')}$$

$$\boldsymbol{L}_0 \equiv i \begin{bmatrix} \Gamma_L - \Gamma_R & -2\Gamma_L \\ -2\Gamma_R & -(\Gamma_L - \Gamma_R) \end{bmatrix},$$

$$\left\{ \boldsymbol{G}_{0,m}(\omega) \right\}^{-1} = (\omega - \epsilon_{d,m})\, \boldsymbol{\tau}_3 + i\Delta[\,1 - 2 f_{\rm eff}(\omega)\,](\mathbf{1} - \boldsymbol{\tau}_1) - \Delta \boldsymbol{\tau}_2$$

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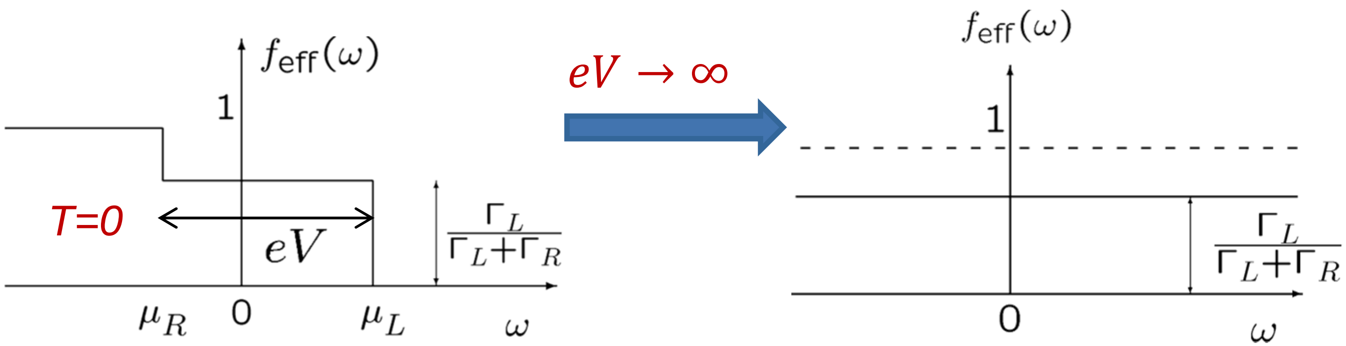
eV and T enter through

$$f_{\rm eff}(\omega) = \frac{f_L(\omega)\,\Gamma_L + f_R(\omega)\,\Gamma_R}{\Gamma_L + \Gamma_R}$$

$$f_\alpha(\omega) = f(\omega - \mu_\alpha),\qquad \alpha = L,\ R$$

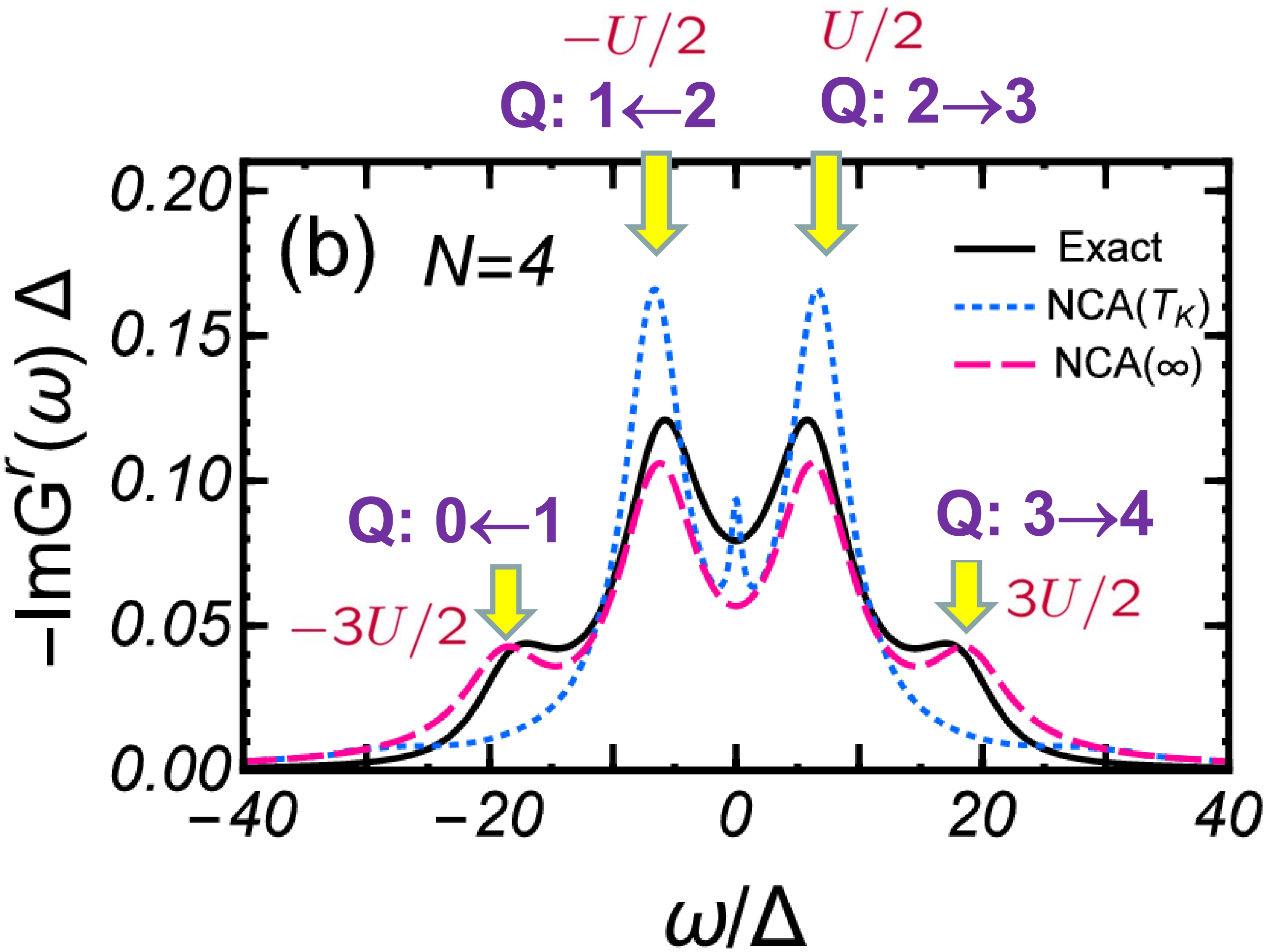
A.O, JPSJ (2002)



Excitations of all energy scales contribute with an equal weight

NCA ($T \to \infty$, dashed), NCA ($T = T_K$, dotted) & Exact $T \to \infty$ limit (solid)

High & *Intermediate temperature results at half-filling*:



$$\frac{U}{\Delta} = 4\pi$$

Transition from 2-peak to 4-peak structure occurs at $T \sim U$

Low temperature properties

1/(N-1) expansion *&* *NRG*

Two different *large* *N* approaches

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1. *Conventional Theory* (NCA, …):

Atomic limit + perturbation expansion in *hybridization* *v*

works mainly for $T \gtrsim T_K$.

2. *Our approach*: 1/(N-1) *expansion*,

HF solution + perturbation expansion in *Coulomb repulsion* *U*

works for low-energy Fermi-liquid region at $T \lesssim T_K$

Our approach uses another kind of standard large N prescription
for two-body interactions, such as the one used for the ϕ^4 *model*

Conventional large *N* theory:

Atomic limit + *perturbation expansion in Hybridization v*

- *Example*: *resolvent self-energy for an empty impurity state,*

$$\Sigma_e = \sum_{k=1}^{\infty} A_{2k}\, v^{2k} = \sum_{k=1}^{\infty} \left(\sum_{p=0}^{k-1} A_{2k}^{(k-p)} \frac{1}{N^p} \right) \left\{ N v^2 \right\}^k$$

scaling: Nv^2 = *const* for $N \to \infty$

$$A_{2k} = \sum_{m=1}^{k} A_{2k}^{(m)} N^m = \underbrace{A_{2k}^{(k)} N^k}_{} + \underbrace{A_{2k}^{(k-1)} N^{k-1}}_{} + \cdots,$$

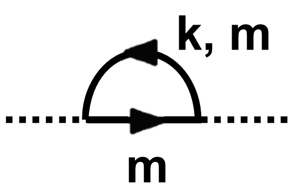
polynomial of N of order k

Leading order in N

Next leading order in N

Leading order approximation: *keeps* $A_{2k}^{(k)}$ *only* (*for all* k)

Next leading order approximation: *keeps* $A_{2k}^{(k)}$ *and* $A_{2k}^{(k-1)}$ *for all* k



Diagrams for the resolvent can be classified according to the number of loops, each of which gives a factor of N

Basic idea of 1/(*N* -1) expansion

[R.Sakano, T.Fujii, & A.O, PRB 83 (2011)]

- *Example: perturbation expansion in U for the vertex correction*

$$u \equiv \frac{U}{\pi\Delta}$$

$$\frac{1}{\pi\Delta}\Gamma_{mm';m'm}(0,0;0,0) = u-(N-2)u^2+\left[N^2-\left(\frac{\pi^2}{2}-1\right)N+9-\frac{\pi^2}{2}\right]u^3$$
$$(m \neq m')$$
$$-(N-2)\left[N^2-\left(12+\frac{7}{4}\pi^2-21\zeta(3)\right)N-17-\frac{71}{12}\pi^2+\frac{133}{2}\zeta(3)\right]u^4+\cdots,$$

$$= \sum_{k=1}^{\infty} C_k\, u^k$$

← *polynomial of* (*N-1*) *of order* *k-1*.

$$C_k = \sum_{m=0}^{k-1} C_k^{(m)}(N-1)^m = \underbrace{C_k^{(k-1)}(N-1)^{k-1}}_{\text{Leading order in }(N-1)} + \underbrace{C_k^{(k-2)}(N-1)^{k-2}}_{\text{Next leading order in }(N-1)} + \cdots,$$

Leading order in (*N* -1)

Next leading order in (*N* -1)

Leading order approximation: *keeps* $C_{2k}^{(k-1)}$ *only* (*for all* k)

Next leading order approximation: *keeps* $C_{2k}^{(k-1)}$ *and* $C_{2k}^{(k-2)}$ *for all* k

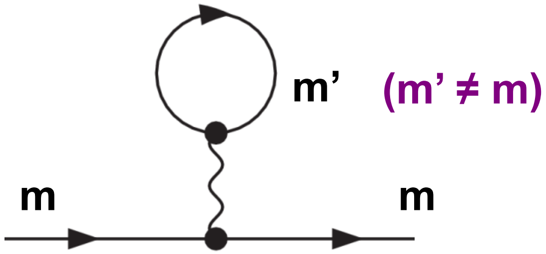
$$\frac{1}{\pi\Delta}\Gamma_{mm';m'm}(0,0;0,0) = \sum_{k=1}^{\infty}\sum_{p=1}^{k} C_k^{(k-p)}\left(\frac{1}{N-1}\right)^p \{(N-1)u\}^k$$

scaling: *(N-1)U = const* *for* *N*→ ∞

Zero order in 1/(N-1) expansion: Hartree-Fock approximation

$$E_d = \epsilon_d + (N-1)\,U\,\langle n_{dm'} \rangle \ ,$$

*(N-1)U is a natural **scaling** parameter for the Coulomb interaction of the SU(N) impurity.*

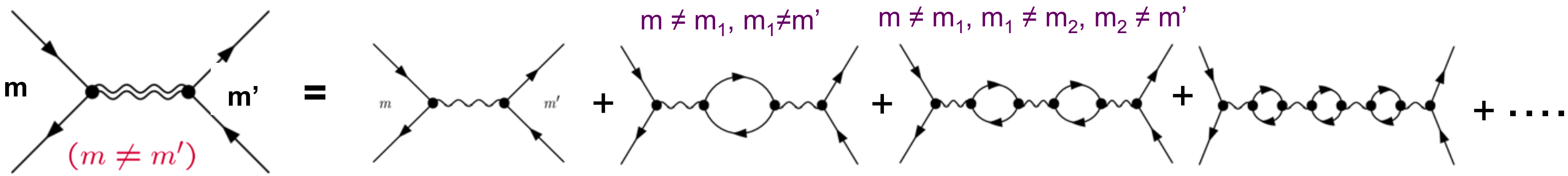


Fermion loop gives a factor of N -1, the number of interacting orbitals, excluding one prohibited by m' ≠ m.

$$g \equiv \frac{(N-1)U}{\pi\Delta}$$

Order 1/(N-1) corrections:

Leading order contributions in the 1/(*N* -1) expansion describes HF-RPA



*Each bubble gives a factor of **order** N-1*

A.O., R. Sakano, & T. Fujii, PRB 84 (2011)

$1/(N\text{-}1)$ expansion ***away from half-filling*** (2nd step)

Perturbative renormalization of the impurity level :

$$\mathcal{H}_d = \sum_{m=1}^{N} \epsilon_d \, n_{dm} + \frac{U}{2} \sum_{\substack{m,\, m' \\ (m \neq m')}} n_{dm} \, n_{dm'} \,,$$

$$= \underbrace{\sum_{m=1}^{N} E_d^* \, n_{dm}}_{E_d^* \equiv E_d + \Sigma(0)\,,} \; \underbrace{- \sum_{m=1}^{N} \lambda \, n_{dm} + \frac{U}{2} \sum_{\substack{m,\, m' \\ (m \neq m')}} \big[n_{dm} - \langle n_{dm} \rangle \big] \big[n_{dm'} - \langle n_{dm'} \rangle \big]}_{\mathcal{H}_I^*} + \text{const.}\,,$$

$$E_d = \epsilon_d + (N-1) U \langle n_{dm} \rangle \,,$$

Perturbation part includes the ***counter term***:

$$\lambda \equiv \Sigma(0) \,,$$

Green's function: $G_0(i\omega) = \dfrac{1}{i\omega - E_d^* + i\Delta \,\text{sgn}\, \omega}$, $\quad G(i\omega) = \dfrac{1}{i\omega - E_d^* + i\Delta \,\text{sgn}\, \omega - \Sigma_{\text{rem}}(i\omega)}$,

Friedel sum rule: $\langle n_{dm} \rangle = \dfrac{1}{\pi} \cot^{-1} \left(\dfrac{E_d^*}{\Delta} \right)$,

Self-energy due to $\mathcal{H}_I^*$: $\Sigma_{\text{rem}}(i\omega) = \Sigma(i\omega) - \Sigma(0)$,

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$\Sigma_{\text{rem}}(i\omega)$ is calculated as a function of E_d^* and λ.

These parameters are determined by the conditions:

$$\begin{cases} \Sigma_{\text{rem}}(0) = 0 \,, \\ E_d^* = \epsilon_d + \Delta \, g \cot^{-1} \left(\dfrac{E_d^*}{\Delta} \right) + \lambda \,, \end{cases}$$

A.O., PRB 85 (2012)

Next leading order terms: *fluctuations beyond the HF+RPA*

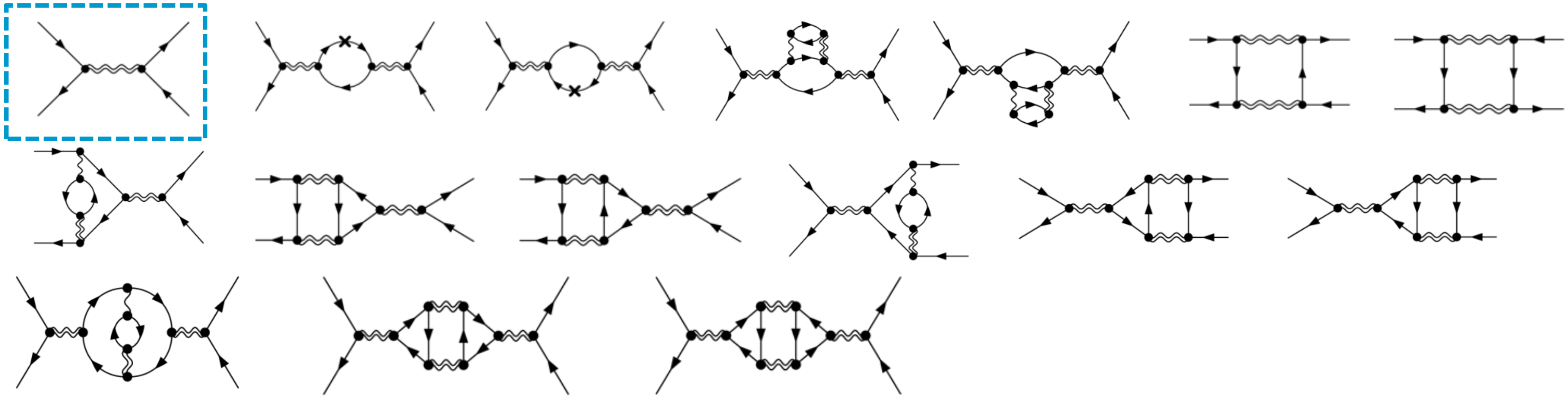
Zero order : Hartree-Fock (HF),

Leading order in $1/(N-1)$: HF-RPA,

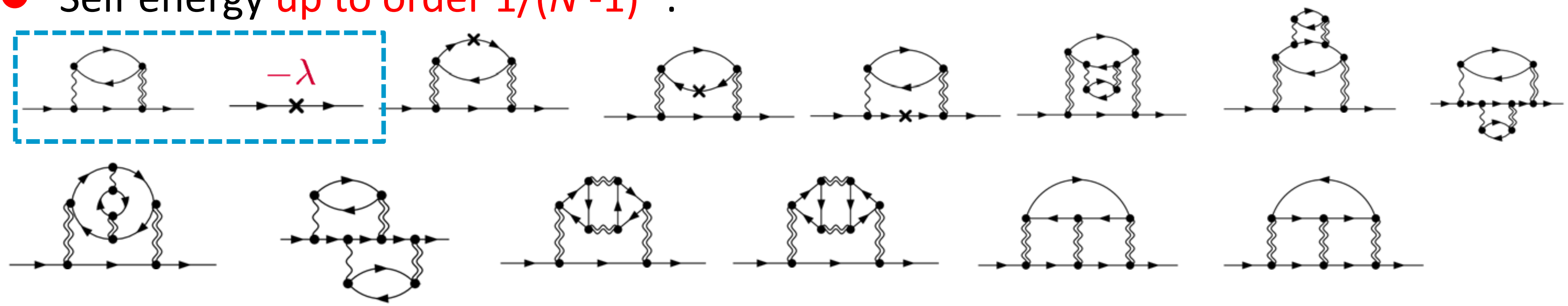
counter term: $\lambda \equiv \Sigma(0)$,

$E_d^* \equiv E_d + \Sigma(0)$,

- Vertex corrections up to order $1/(N-1)^2$:



- Self energy up to order $1/(N-1)^2$:



A.O., PRB 85 (2012)

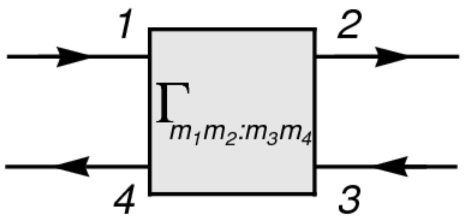
Local Fermi-liquid parameters

Green's function: $$G_m(\omega) = \frac{1}{\omega - E_d + i\Delta - \Sigma_m(\omega)} ,$$

$$E_d \equiv \epsilon_d + (N-1)U\langle n_{dm}\rangle ,$$

$$Z^{-1} \equiv 1 - \left.\frac{\partial \Sigma(\omega)}{\partial \omega}\right|_{\omega=0} ,$$

Vertex corrections:



$$\Gamma_{m_1,m_2;m_3,m_4}(\omega_1,\omega_2;\omega_3,\omega_4)$$

$$\widetilde{U} \equiv Z^2\Gamma_{mm';m'm}(0,0;0,0)$$

$$(m \neq m')$$

Low-energy properties are determined by $\Sigma(\omega)$ *and* $\Gamma_{mm';m'm}(\omega,\omega';\omega',\omega)$ *for* ***small*** ω, *and can be characterized by the three renormalized parameters*:

Width of Kondo resonance: $\widetilde{\Delta} = Z\Delta \sim T_K,$

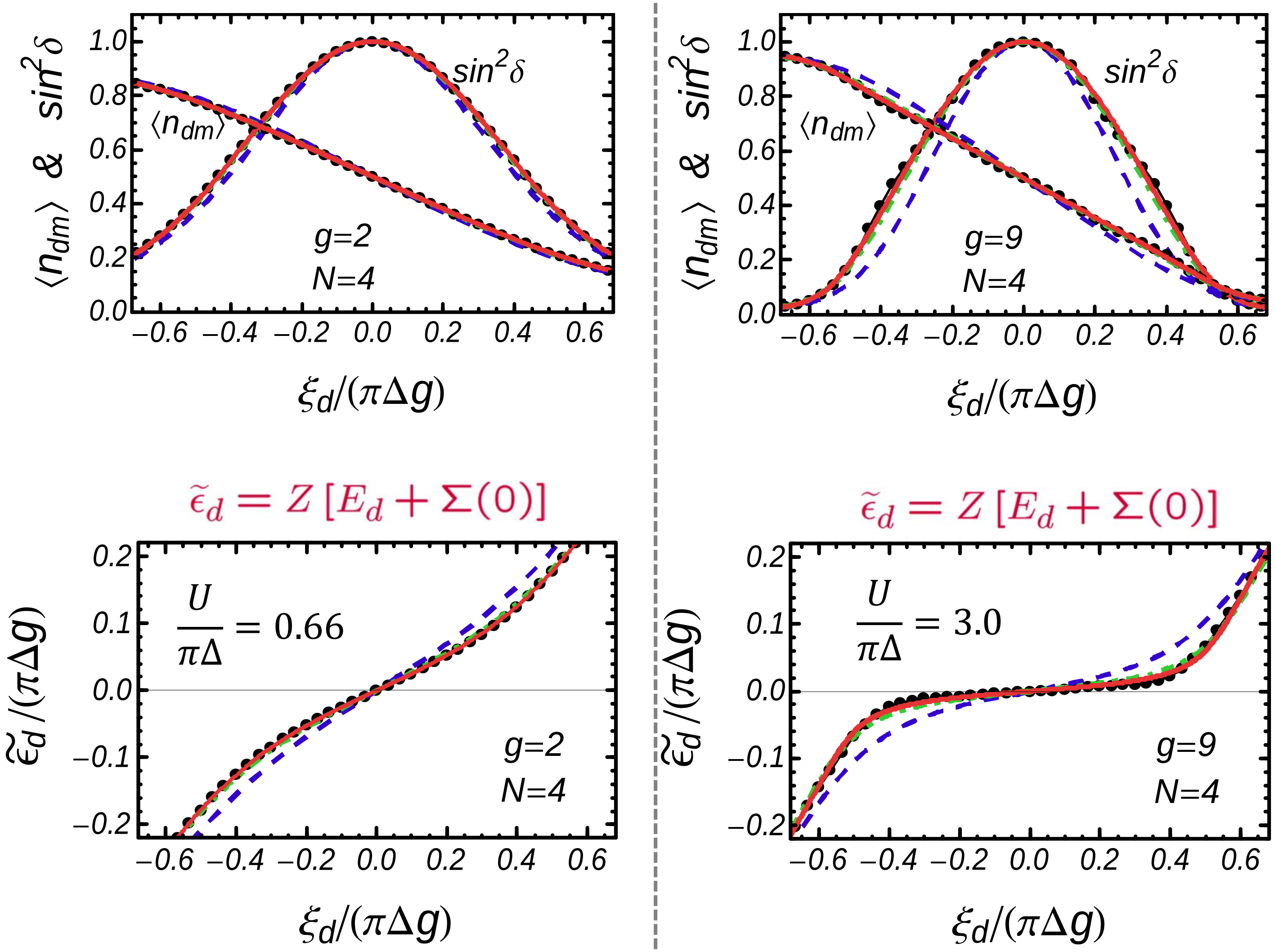
Wilson ratio: $R = 1 + \dfrac{\widetilde{U}}{\pi\widetilde{\Delta}} ,$

Renormalized impurity level: $\widetilde{\epsilon}_d = Z\left[E_d + \Sigma(0)\right] ,$

Next leading order results for $N = 4$: *away from half-filling*

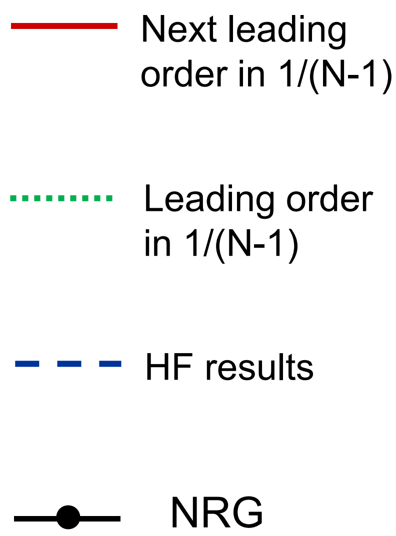
"Small U", $\frac{U}{\pi\Delta} = 0.66$

"Large U", $\frac{U}{\pi\Delta} = 3.0$



$$g \equiv \frac{(N-1)U}{\pi\Delta}$$

$$\xi_d \equiv \epsilon_d + \frac{U(N-1)}{2}$$



$$\langle n_{dm}\rangle = \frac{\delta}{\pi}$$

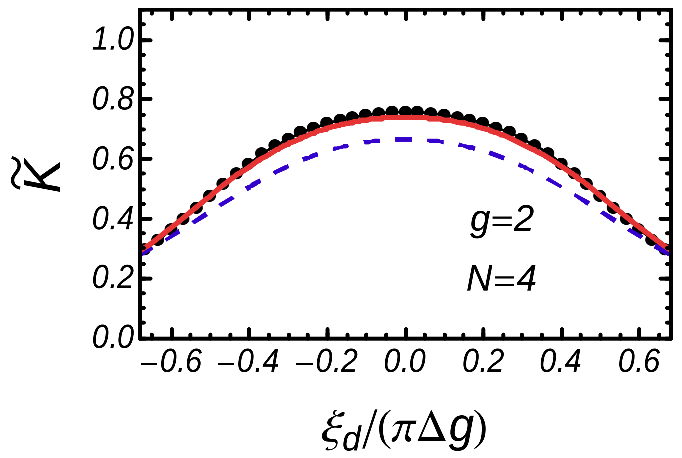
$$G^r(0) = -\frac{\sin\delta}{\Delta}\, e^{i\delta}$$

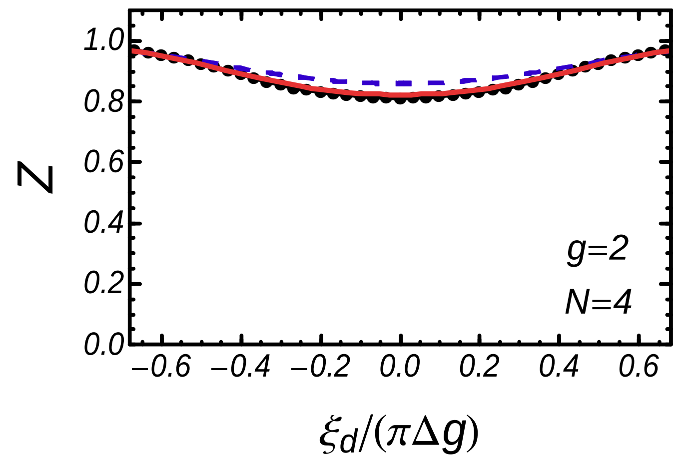
A.O., PRB 85 (2012)

Next leading order results of Z & R for $N = 4$: *away from half-filling*

"Small U", $U/(\pi\Delta) = 0.66$

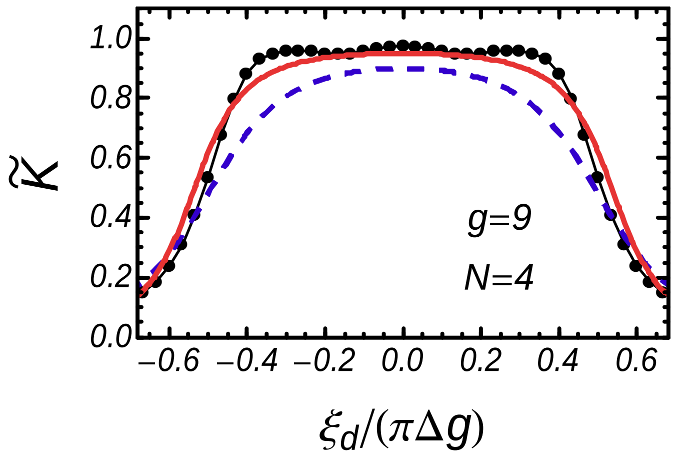
$$\widetilde{K} = (N-1)(R-1)$$

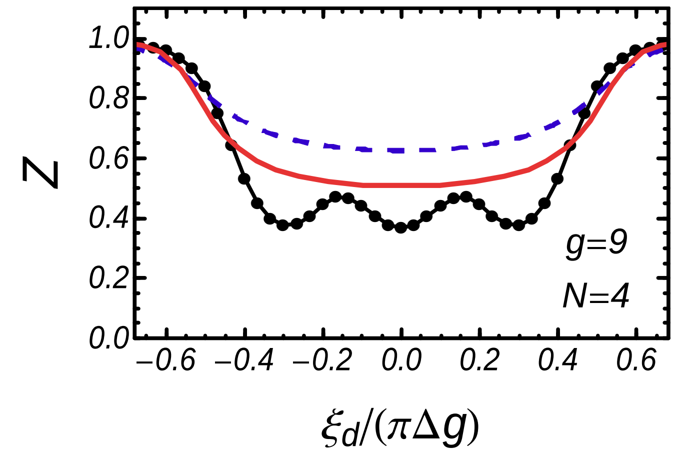




"Large U", $U/(\pi\Delta) = 3.0$

$$\widetilde{K} = (N-1)(R-1)$$





$$g \equiv \frac{(N-1)U}{\pi\Delta},$$

$$\xi_d \equiv \epsilon_d + \frac{U(N-1)}{2},$$

Next leading order in 1/(N-1)

Leading order in 1/(N-1)

NRG

$$\widetilde{K} \equiv \frac{(N-1)\widetilde{U}}{\pi\widetilde{\Delta}} \sin^2\delta$$

$$R = 1 + \frac{\widetilde{K}}{N-1}$$

$$0 \leq \widetilde{K} < 1,$$

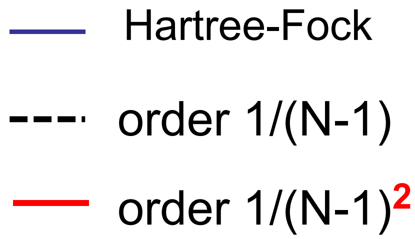
Order $1/(N-1)^2$ & NRG results of Green's function

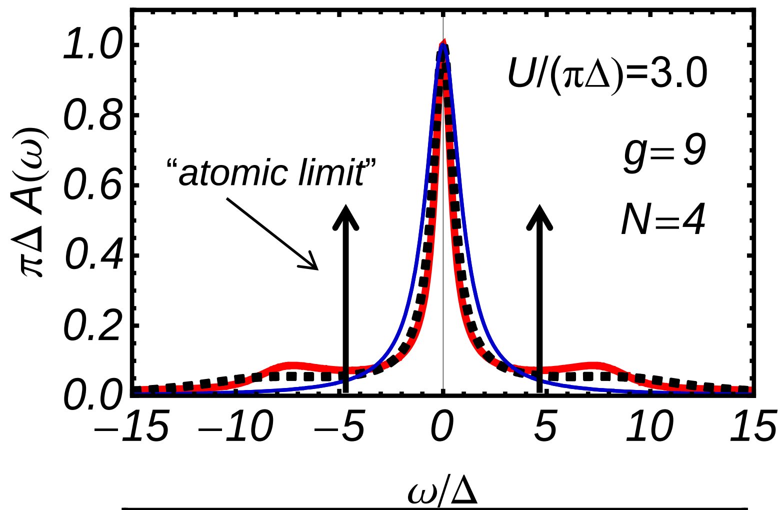
in the electron-hole symmetric case

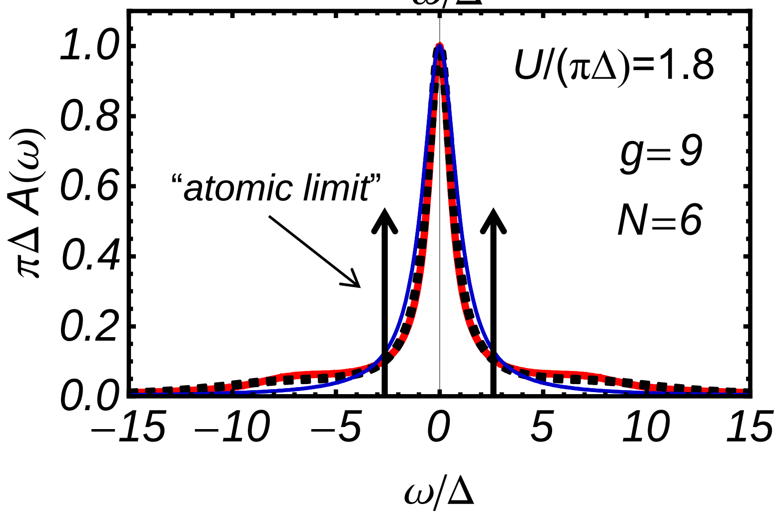
Order $1/(N-1)^2$ results of $G(\omega)$ for $T=0$ and $g=9$:

$$g \equiv \frac{(N-1)U}{\pi\Delta}$$

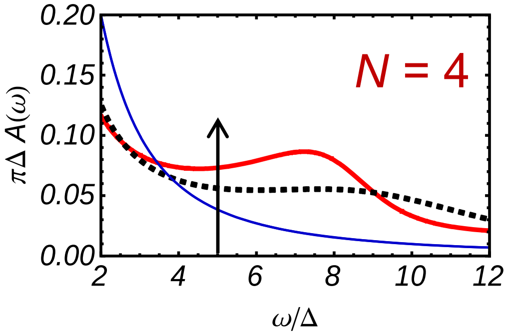
$$A(\omega) = -\frac{1}{\pi}\,\mathrm{Im}\,G^r(\omega)$$ *at half-filling*

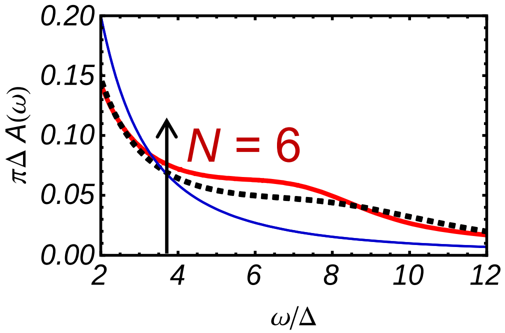






"Sub peak structure"





- ***For fixed g,*** *electron correlation is suppressed as* ***N*** *increases.*

A.O, M. Awane, & R. Sakano.

Summary

Green's function & Local-Fermi-liquid parameters for SU(N) Anderson impurity:

- Exact Green's function at $eV \to \infty$ captures the imaginary part due to multiple particle-hole pair excitations (*relaxation process at high-energy scale*)

- Exact $T \to \infty$ result describes the higher-frequency sub-peak structure.
  Finite-U NCA describes T-dependence of the sub-peak structure at $T \gtrsim U$.

- 1/(N -1) expansion based on a perturbation theory in U correctly describes the low-energy Fermi-liquid properties, and agree with the NRG results for small couplings $g \equiv \frac{(N-1)U}{\pi\Delta}$ *and* ω.

  Possible extensions: *Non-equilibrium Green's function,*
  Application to bulk electrons (*Hubbard model, DMFT, etc.*).