12th International Conference on the Exact RG

22.-27. September 2024, Les Diablerets

Recursive algorithm for generating high-temperature expansions for spin systems and the chiral non-linear susceptibility

Peter Kopietz, Frankfurt

with A. Rückriegel, D. Tarasevych, J. Krieg

arXiv: 2406.06270, to appear in PRB

1. Spin diagram technique
2. Spin-FRG
3. High-T expansion from Spin-FRG
4. Chiral non-linear susceptibility

1. Spin diagram technique

Basic idea: Vaks, Larkin, Pikin 1968:

work directly with physical spin-S operators, no unphysical states, no projections, no redundancy in Hilbert space

VLP 1:
Wick theorem for spin operators, spin-diagram technique, thermodynamics

SOVIET PHYSICS JETP VOLUME 26, NUMBER 1 JANUARY, 1968

THERMODYNAMICS OF AN IDEAL FERROMAGNETIC SUBSTANCE

V. G. VAKS, A. I. LARKIN, and S. A. PIKIN

Submitted February 1, 1967

Zh. Eksp. Teor. Fiz. 53, 281–299 (July, 1967)

A diagram technique is proposed for a system of interacting spins which permits one to study the thermodynamics of a Heisenberg ferromagnet with arbitrary spin S at any temperature T or magnetic field strength H. The relevant high-temperature expansions are presented. Ex-

VLP 2:
spin waves, correlation functions

SOVIET PHYSICS JETP VOLUME 26, NUMBER 3 MARCH, 1968

SPIN WAVES AND CORRELATION FUNCTIONS IN A FERROMAGNETIC

V. G. VAKS, A. I. LARKIN, and S. A. PIKIN

Submitted April 6, 1967

Zh. Eksp. Teor. Fiz. (U.S.S.R.) 53, 1089–1106 (September, 1967)

We consider the spin waves and correlation functions in a Heisenberg ferromagnet in the complete temperature range below the transition temperature T_c. We find the damping of the spin waves and

complicated diagrammatics for quantum spin systems

- strategy: expand in powers of J_{ij}
- generalized Wick theorem for spin operators requires several types of vertices:

(from book by Izyumov and Skryabin, 1988)

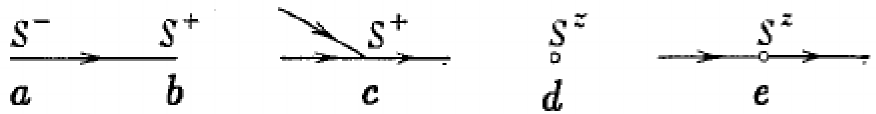
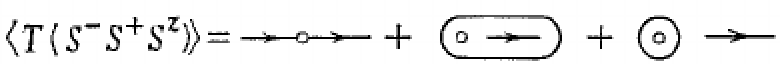
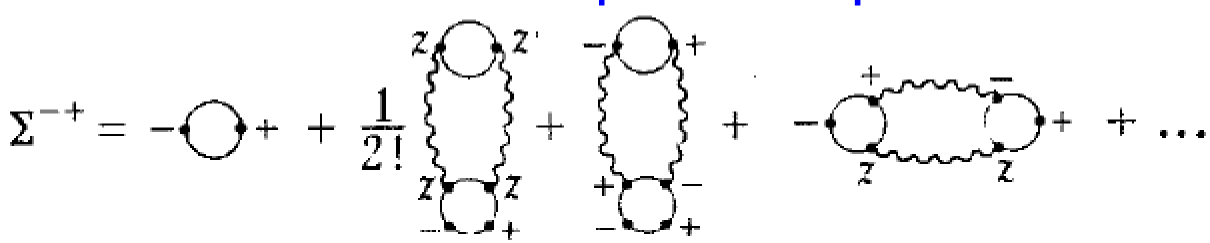


Fig. 2.1. Types of vertices for the exchange Hamiltonian. (For convenience vertices of types *d* and *e* are denoted by hollow bullets.)



- expansion of irreducible part of 2-point function in powers of J_{ij}



- complicated diagrammatics → method not very popular

(see, however, talk by B. Sbierski this conference and B. Schneider, …, B. Sbierski, arXiv: 2407.18156)

- reformulate in framework of FRG → SFRG (Spin FRG)

2. Spin FRG

- Krieg, PK, PRB 2019 (original idea, see ERG 2018, Paris)
- Tarasevych, Krieg, PK, PRB 2018 (Kondo-problem)
- Goll, Tarasevych, Krieg, PK, PRB 2019 (Heisenberg ferromagnets)
- Goll, Rückriegel, PK, PRB 2020 (zero-magnon sound)
- Tarasevych, PK, PRB 2021 (high-temperature spin dynamics in paramagnets)
- Tarasevych, PK, PRB 2022 (critical spin dynamics in ferromagnets)
- Rückriegel, Arnold, Goll, PK, PRB 2022 (dimerized spin systems)
- Tarasevych et al., PRB 2022 (J1J2J3 model)
- Rückriegel, Arnold, Krämer, PK, PRB 2023 (X-operators)
  (see poster by Jonas Arnold this conference)
- Rückriegel, Tarasevyh, PK, (J1J2 model in 2d)
  (see talk by Andreas Rückriegel this conference)
- Rückriegel, Tarasevych, Krieg, PK, (high-T expansions)

SFRG: basic idea

- general anisotropic Heisenberg model

$$\mathcal{H} = \frac{1}{2}\sum_{ij}\sum_{ab} J_{ij}^{ab} S_i^a S_j^b \; + \; \mathcal{H}_0 \qquad\qquad \mathcal{H}_0 \; = -\sum_i H_i S_i^z$$

- deform exchange interaction

$$J_{ij}^{ab} \to \; J_{ij,\Lambda}^{ab} = J_{ij}^{ab} + R_{ij,\Lambda}^{ab}$$

- example: interaction switch

$$J_{ij,\Lambda}^{ab} = \Lambda J_{ij}^{ab}, \quad \Lambda \in [0,1]$$

- generating functional of connected imaginary-time ordered correlation functions

$$e^{\mathcal{G}_\Lambda[\boldsymbol{h}]} = \mathrm{Tr}\left\{ e^{-\beta\mathcal{H}_0} \mathcal{T} e^{\int_0^\beta d\tau \sum_i \boldsymbol{h}_i(\tau)\cdot\boldsymbol{S}_i(\tau)} e^{-\int_0^\beta d\tau \frac{1}{2}\sum_{ij}\sum_{ab} J_{ij,\Lambda}^{ab} S_i^a(\tau) S_j^b(\tau)} \right\}$$

- satisfies exact flow equation (Krieg+PK 2019)

$$\partial_\Lambda \mathcal{G}_\Lambda[\boldsymbol{h}] = -\frac{1}{2}\int_0^\beta d\tau \sum_{ij,ab} (\partial_\Lambda J_{ij,\Lambda}^{ab}) \left[\frac{\delta^2 \mathcal{G}_\Lambda[\boldsymbol{h}]}{\delta h_i^a(\tau)\delta h_j^b(\tau)} + \frac{\delta \mathcal{G}_\Lambda[\boldsymbol{h}]}{\delta h_i^a(\tau)} \frac{\delta \mathcal{G}_\Lambda[\boldsymbol{h}]}{\delta h_j^b(\tau)} \right]$$

Wetterich equation for quantum spins

- subtracted Legendre transform

$$\Gamma_\Lambda[\boldsymbol{M}] = \int_0^\beta d\tau \sum_i \boldsymbol{h}_i(\tau) \cdot \boldsymbol{M}_i(\tau) - \mathcal{G}_\Lambda[\boldsymbol{h}] - \frac{1}{2} \int_0^\beta d\tau \sum_{ij} R_{ij}^\Lambda \boldsymbol{M}_i(\tau) \cdot \boldsymbol{M}_j(\tau)$$

- bosonic Wetterich equation for quantum spin systems

$$\partial_\Lambda \Gamma_\Lambda[\boldsymbol{M}] = \frac{1}{2} \mathrm{Tr} \left\{ \left(\boldsymbol{\Gamma}''_\Lambda[\boldsymbol{M}] + \mathbf{R}_\Lambda \right)^{-1} \partial_\Lambda \mathbf{R}_\Lambda \right\}$$

spin algebra hidden in initial conditions!

- problem: for quantum spin systems Legendre trafo does not exist at $\Lambda = 0$ if $J^{ab}_{ij,\Lambda=0} = 0$ (first pointed out by Rancon PRB 2014)

- solution: use different types of generating functionals (interaction irreducible or classical-quantum hybrid functionals)

- classical spin systems Wetterich equation can be used to generate high-temperature expansions (Rancon PRE 2016)

- better: start from generating functional of connected correlation functions

3. High-T expansion for spin systems from Spin-FRG

- high-temperature expansions: well developed algorithms available
  Domb+Green Vol.3: Series expansions for lattice models, 1974;
  Oitmaa, Hamer, Zheng, Series expansion method for strongly interacting lattice models, 2006

- here: new algorithm based on exact FRG flow equation
  for connected spin correlation functions

$$\partial_\Lambda \mathcal{G}_\Lambda[\boldsymbol{h}] = -\frac{1}{2}\int_0^\beta d\tau \sum_{ij,ab} (\partial_\Lambda J^{ab}_{ij,\Lambda}) \left[\frac{\delta^2 \mathcal{G}_\Lambda[\boldsymbol{h}]}{\delta h^a_i(\tau)\delta h^b_j(\tau)} + \frac{\delta \mathcal{G}_\Lambda[\boldsymbol{h}]}{\delta h^a_i(\tau)} \frac{\delta \mathcal{G}_\Lambda[\boldsymbol{h}]}{\delta h^b_j(\tau)} \right]$$

- equivalent hierarchy of flow equations:

$$\partial_\Lambda G^{(n)}_{\alpha_1\ldots\alpha_n} = -\frac{1}{2}\int_\alpha \int_{\alpha'} [(\partial_\Lambda \mathbf{J}_\Lambda)]_{\alpha\alpha'} \Big[G^{(n+2)}_{\alpha\alpha'\alpha_1\ldots\alpha_n} + \sum_{m=0}^{n} \mathcal{S}_{1,\ldots,m;m+1,\ldots,n} \left\{ G^{(m+1)}_{\alpha\alpha_1\ldots\alpha_m} G^{(n-m+1)}_{\alpha'\alpha_{m+1}\ldots\alpha_n} \right\} \Big]$$

$$\int_\alpha = \int_0^\beta d\tau \sum_{ia}$$

symmetrization operator: $\mathcal{S}_{1,\ldots,m;m+1,\ldots,n}\{f(1,\ldots,n)\} = \frac{1}{m!(n-m)!}\sum_P f(P_1,\ldots,P_n)$

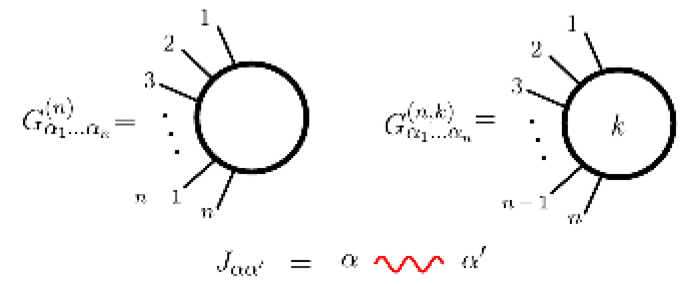
recursion relation from spin FRG

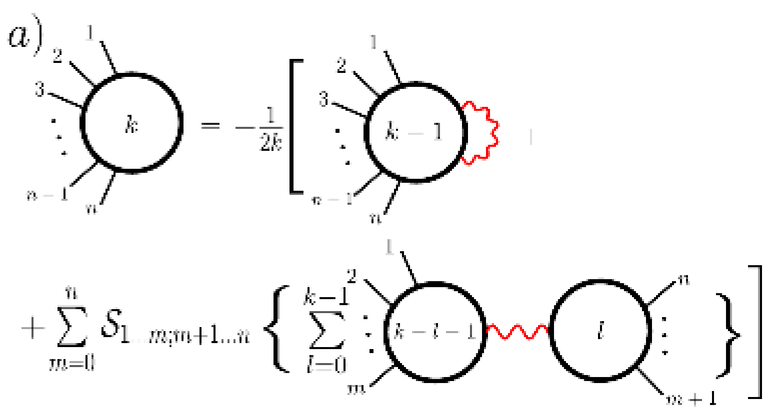
- use flow equation for generating functional of connected correlation functions for high-T expansion (Wetterich equation inconvenient)

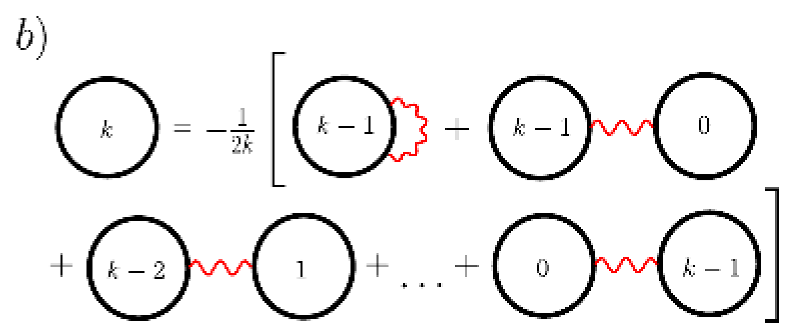
- interaction-switch deformation scheme: $J^{ab}_{ij,\Lambda} = \Lambda J^{ab}_{ij}, \quad \Lambda \in [0,1]$

- expand in powers of switch-parameter: $G^{(n)}_{\alpha_1 \ldots \alpha_n,\Lambda} = \sum_{k=0}^{\infty} \Lambda^k G^{(n,k)}_{\alpha_1 \ldots \alpha_n}$

$$G^{(n,k)}_{\alpha_1 \ldots \alpha_n} = -\frac{1}{2k} \int_\alpha \int_{\alpha'} J_{\alpha\alpha'} \Bigg[G^{(n+2,k-1)}_{\alpha\alpha'\alpha_1 \ldots \alpha_n} + \sum_{m=0}^{n} \mathcal{S}_{1,\ldots,m;m+1,\ldots,n} \left\{ \sum_{l=0}^{k-1} G^{(m+1,l)}_{\alpha\alpha_1 \ldots \alpha_m} G^{(n-m+1,k-l-1)}_{\alpha'\alpha_{m+1} \ldots \alpha_n} \right\} \Bigg]$$





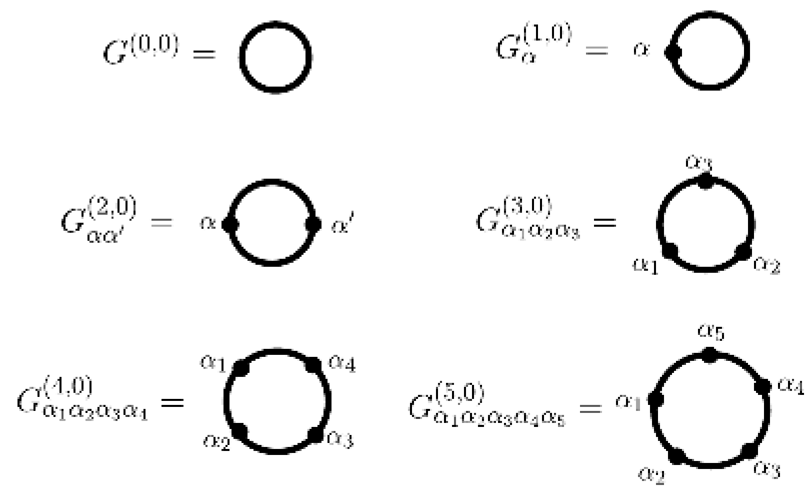


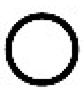
generalized blocks

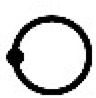
- iteration reproduces all terms of spin diagram technique without using generalized Wick-theorem for spin operators

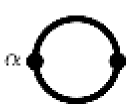
- zeroth-order: generalized blocks:

  non-trivial functions of external frequencies (due to spin algebra)

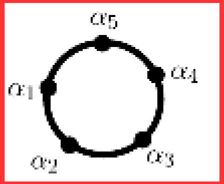


$G^{(0,0)} =$  $= \sum_i B(\beta H_i)$ $\qquad B(y) = \ln\left[\frac{\sinh[(S+1/2)y]}{\sinh(y/2)}\right]$

$G^{(1,0)}_{\alpha} = \alpha$  $= \; m_i = b(\beta H_i).$ $\qquad b(y) = \left(S+\frac{1}{2}\right)\coth\left[\left(S+\frac{1}{2}\right)y\right] - \frac{1}{2}\coth\left[\frac{y}{2}\right]$

$G^{(2,0)}_{\alpha\alpha'} = \alpha$  α' $\qquad g_i^{zz}(\omega) = \beta\delta_{\omega,0}b'(\beta H_i)$ $\qquad g_i^{+-}(\omega) = g_i^{-+}(-\omega) = \frac{m_i}{H_i - i\omega}.$

generalized 5-spin blocks



$$
\begin{aligned}
b^3 g^{++--z}(\omega_1,\omega_2,\omega_3,\omega_4,\omega_5) &= g(-\omega_3)g(-\omega_4)\Big\{ \\
& g(\omega_1)\Big[g(\omega_1+\omega_5)+g(-\omega_3-\omega_5)+g(-\omega_4-\omega_5)-\beta[\delta_{\omega_5,0}+\delta_{\omega_2,-\omega_3}+\delta_{\omega_2,-\omega_4}]b'\Big] \\
& +g(\omega_2)\Big[g(\omega_2+\omega_5)+g(-\omega_3-\omega_5)+g(-\omega_4-\omega_5)-\beta[\delta_{\omega_5,0}+\delta_{\omega_1,-\omega_3}+\delta_{\omega_1,-\omega_4}]b'\Big] \\
& +\beta^2\delta_{\omega_5,0}[\delta_{\omega_1,-\omega_3}+\delta_{\omega_2,-\omega_3}]bb''\Big\},
\end{aligned}
$$

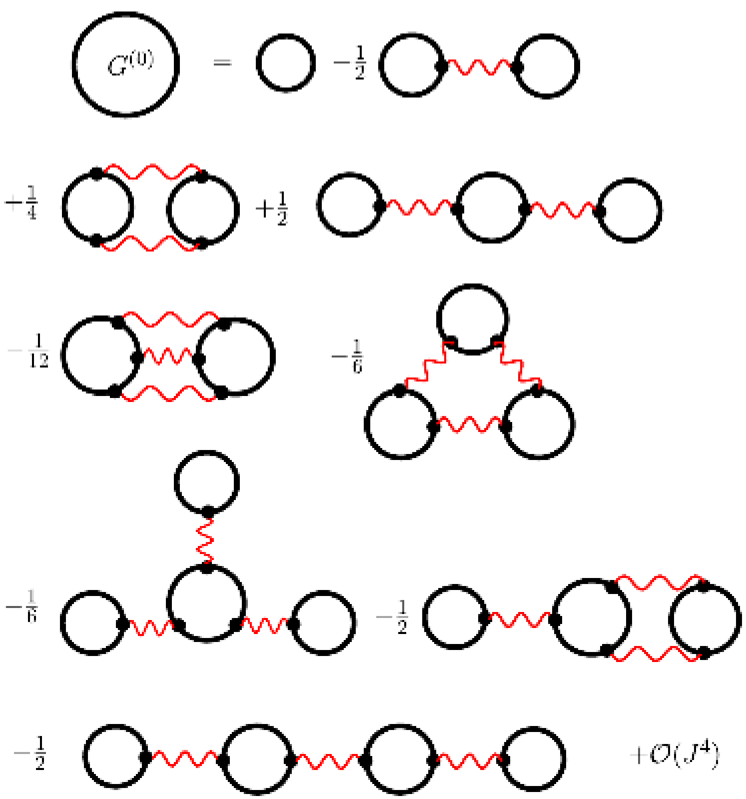
$$
\begin{aligned}
b^3 g^{+-zzz}(\omega_1,\omega_2,\omega_3,\omega_4,\omega_5) &= -g(\omega_1)g(-\omega_2)\Big\{ \\
& \Big[g(\omega_1+\omega_3)-\beta\delta_{\omega_3,0}b'\Big]\Big[g(-\omega_2-\omega_4)+g(-\omega_2-\omega_5)\Big]+\beta^2\delta_{\omega_4,0}\delta_{\omega_5,0}bb'' \\
& +\Big[g(\omega_1+\omega_4)-\beta\delta_{\omega_4,0}b'\Big]\Big[g(-\omega_2-\omega_5)+g(-\omega_2-\omega_3)\Big]+\beta^2\delta_{\omega_5,0}\delta_{\omega_3,0}bb'' \\
& +\Big[g(\omega_1+\omega_5)-\beta\delta_{\omega_5,0}b'\Big]\Big[g(-\omega_2-\omega_3)+g(-\omega_2-\omega_4)\Big]+\beta^2\delta_{\omega_3,0}\delta_{\omega_4,0}bb''\Big\} \\
& +g(-\omega_2)\beta^3\delta_{\omega_3,0}\delta_{\omega_4,0}\delta_{\omega_5,0}b^2b'''.
\end{aligned}
$$

$$
g(\omega)=\frac{b}{H-i\omega},
$$

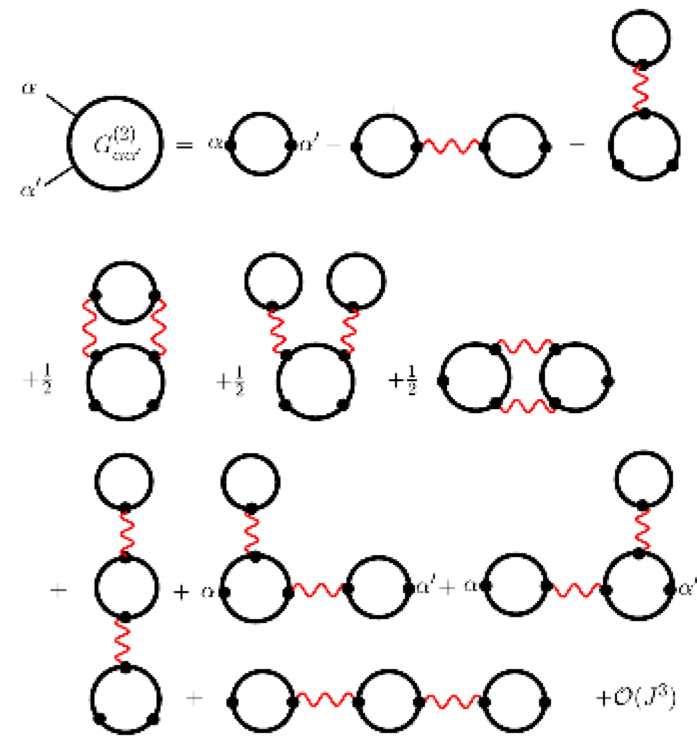
low orders in high-temperature expansions

- straightforward iteration of recursion relation iteration generates first few terms in high-temperature expansion of arbitrary correlation functions

- free energy to third order in J/T:

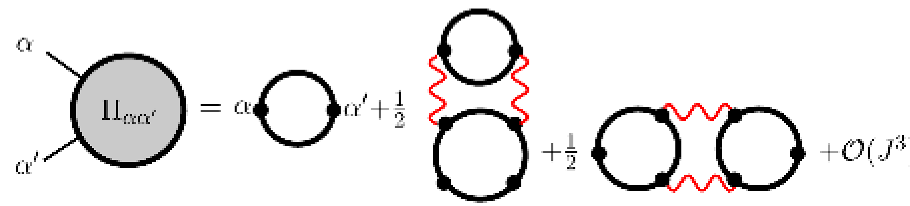


- 2-spin correlation function to 2nd order in J/T:

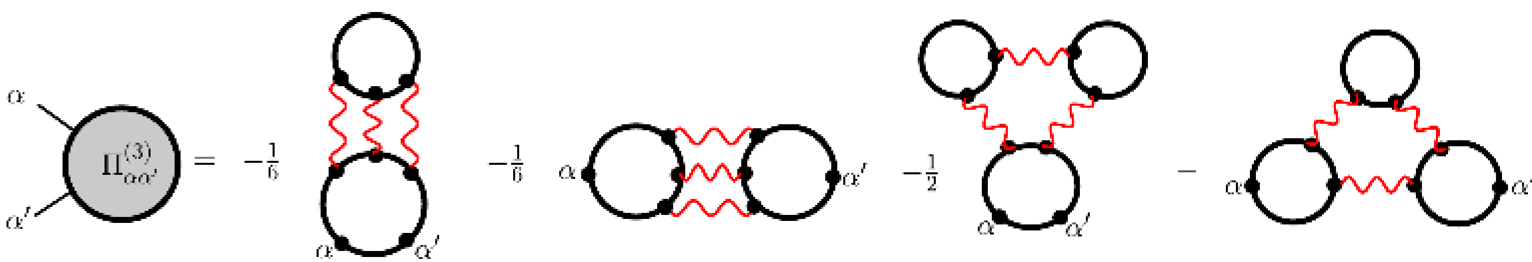


Interaction-irreducible dynamic spin susceptibility

- diagrams up to 2nd order:



- diagrams to 3rd order:

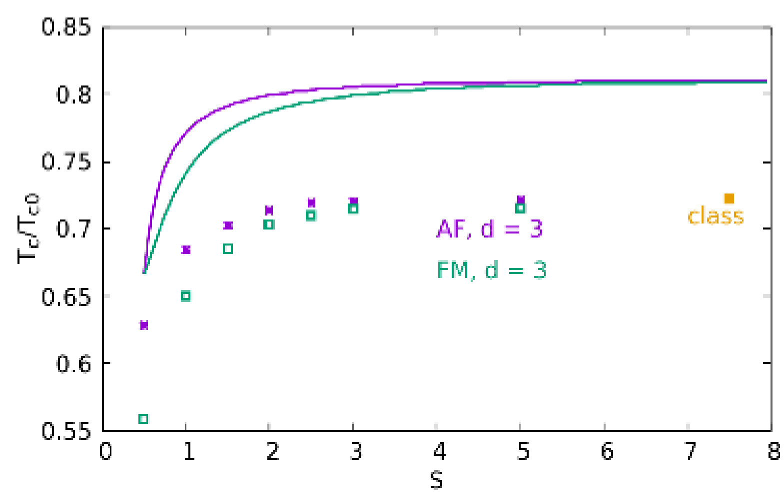


$$= -\delta_{\omega,0}\frac{\beta^4 J_0^3}{(2D)^2}\left[\frac{b_1^2-10b_1b_3}{72}+\frac{(b_1^2+20b_3^2)\gamma_{\boldsymbol{k}}}{72}\right]+(1-\delta_{\omega,0})\frac{\beta^2 J_0^3}{(2D)^2}\frac{b_1^2}{2}\frac{1-\gamma_{\boldsymbol{k}}}{\omega^2}$$

- in paramagnetic regime: estimate critical temperature from

$$J_{\boldsymbol{Q}} + \Pi^{-1}(\boldsymbol{Q},0) = 0.$$

- systematic expansion in 1/D gives better results
(Krieg+PK 2019,
Schneider et al arXiv:2507.18156)



advantage of method

- produces high-temperature expansion of connected spin correlation functions involving arbitrary number of spins within unified formalism

- low orders (up to n=5) can easily be obtained symbolically via MATHEMATICA

- open question: is fully numerical implementaton of algorithm competitive with established algorithms to generate high-order expansions?

4. The chiral non-linear suscepitbility

- connected 3-spin correlation function involving three different spin components
- determines quadratic response to time-dependent magnetic field
- characterizes correlation effects in non-linear response

PHYSICAL REVIEW B **107**, 205108 (2023)

Nonlinear responses and three-particle correlators in correlated electron systems exemplified by the Anderson impurity model

Patrick Kappl, Friedrich Krien, Clemens Watzenböck, and Karsten Held
Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria

(Received 23 December 2022; revised 14 April 2023; accepted 14 April 2023; published 5 May 2023; corrected 26 June 2023)

Three-particle correlators are relevant for, among others, Raman, Hall, and nonlinear responses. They are also required for the next order of approximations extending dynamical mean-field theory diagrammatically. We present a general formalism on how to treat these three-particle correlators and susceptibilities, and we calculate the local three-particle response of the Anderson impurity model numerically. We find that genuine three-particle vertex corrections are sizable. In particular, it is not sufficient to just take the bare bubble terms or corrections based on the two-particle vertex. The full three-particle vertex must be considered.

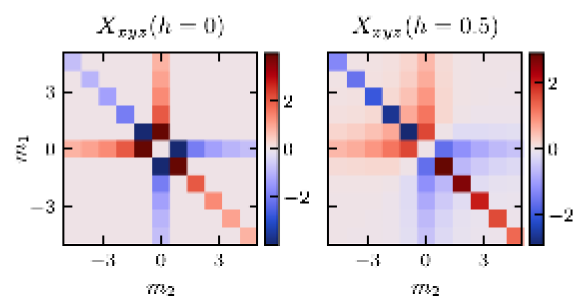
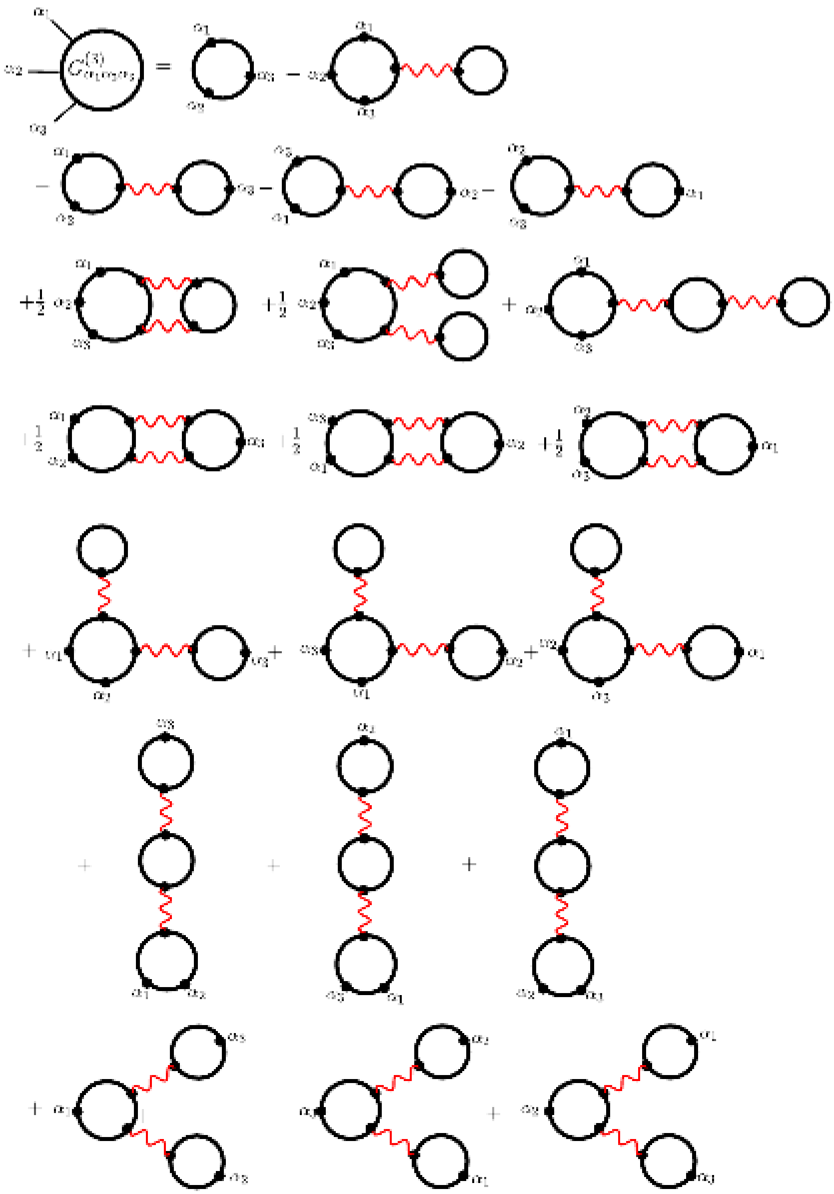


FIG. 4. Full three-particle correlator with flavors x, y, z drawn as a function of the two indices $m_{i=1,2}$ of the bosonic Matsubara frequencies $\omega_i = m_i 2\pi T$; $U = \epsilon = 0$, $\beta = 5$. In the atomic limit, only this flavor combination retains a frequency structure due to noncommutativity of the spin operators. Left: no magnetic field. Right: magnetic field in the z-direction, $h = 0.5$.

- for isolated spin (generalized 3-spin block)   Tarasevych, Krieg, PK, PRB 2018

$$g_0^{a_1 a_2 a_3}(\omega_1,\omega_2,\omega_3) = \epsilon^{a_1 a_2 a_3}\beta b_1\left(1-\delta_{\omega_1,0}\delta_{\omega_2,0}\delta_{\omega_3,0}\right)\left[\frac{\delta_{\omega_1,0}}{\omega_2}+\frac{\delta_{\omega_2,0}}{\omega_3}+\frac{\delta_{\omega_3,0}}{\omega_1}\right]$$

expansion up to 3rd order



$$G^{xyz(1)}(K_1, K_2, K_3) = -\beta^2 b_1^2 (1 - \delta_{\omega_1,0}\delta_{\omega_2,0}\delta_{\omega_3,0}) \times \left[J_{\boldsymbol{k}_1} \frac{\delta_{\omega_1,0}}{\omega_2} + J_{\boldsymbol{k}_2} \frac{\delta_{\omega_2,0}}{\omega_3} + J_{\boldsymbol{k}_3} \frac{\delta_{\omega_3,0}}{\omega_1} \right]$$

$$G^{xyz(2)}(K_1, K_2, K_3) = \beta b_1^2 \left(\frac{1}{N} \sum_{\boldsymbol{q}} J_{\boldsymbol{q}}^2 \right) \times \left[\frac{1-\lambda_{\boldsymbol{k}_1}}{\omega_1^2} \left(\frac{1}{\omega_2} - \frac{1}{\omega_3} \right) + \frac{1-\lambda_{\boldsymbol{k}_2}}{\omega_2^2} \left(\frac{1}{\omega_3} - \frac{1}{\omega_1} \right) + \frac{1-\lambda_{\boldsymbol{k}_3}}{\omega_3^2} \left(\frac{1}{\omega_1} - \frac{1}{\omega_2} \right) \right]$$

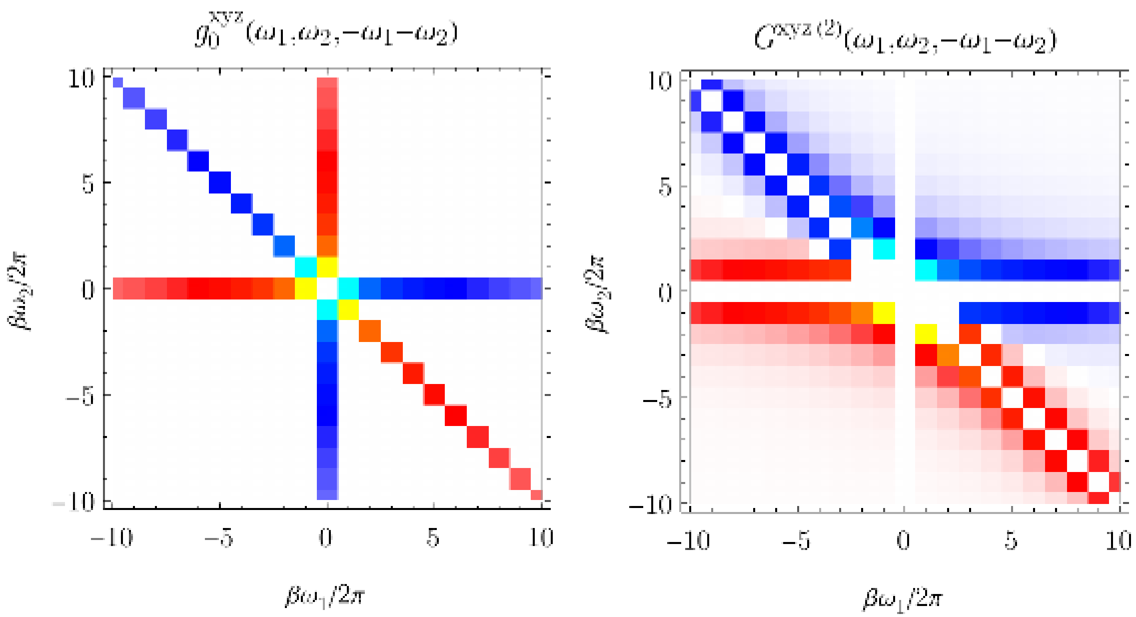
$$\lambda_{\boldsymbol{k}} = \frac{\sum_{\boldsymbol{q}} J_{\boldsymbol{q}} J_{\boldsymbol{q}+\boldsymbol{k}}}{\sum_{\boldsymbol{q}} J_{\boldsymbol{q}}^2}$$

2^{nd} harmonic generation in non-linear response at high frequencies

- possible in 2^{nd} order chiral non-linear susceptibility:

$$G^{xyz(2)}(\boldsymbol{k}_1, \omega, \boldsymbol{k}_2, \omega, -\boldsymbol{k}_1 - \boldsymbol{k}_2, -2\omega) = -3\beta b_1^2 \left(\frac{1}{N} \sum_{\boldsymbol{q}} J_{\boldsymbol{q}}^2 \right) \frac{\lambda_{\boldsymbol{k}_1} - \lambda_{\boldsymbol{k}_2}}{2\omega^3}$$

- full frequency dependence appears in 2^{nd} order:



conclusions+outlook

- High-temperature expansions for correlation functions of quantum spin systems can be obtained using FRG flow equation of generating functional of connected spin correlation functions
- Method is particularly useful for higher-order correlations functions
- Open problem: is fully numerical implementation of recursive algorithm competitive with established methods to generate high orders?
- Method can be generalitzed to obtain high-temperature andstrong-coupling expansions for Hubbard- and tJ-models using generalization of Spin-FRG to Hubbard X-operators: X-FRG
  (Rückriegel et al, PRB 2023; see also Poster by Jonas Arnold this conference)