Cluster Functional Renormalization Group

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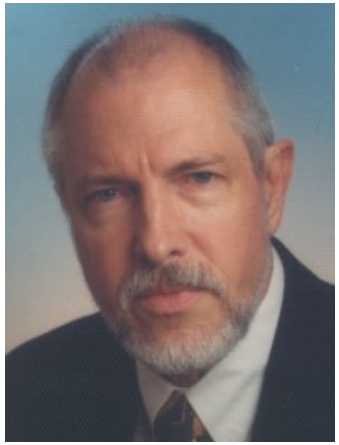
California Institute of Technology (Pasadena)

Lefkada, September 26, 2014

Collaborators

Ronny Thomale
Würzburg



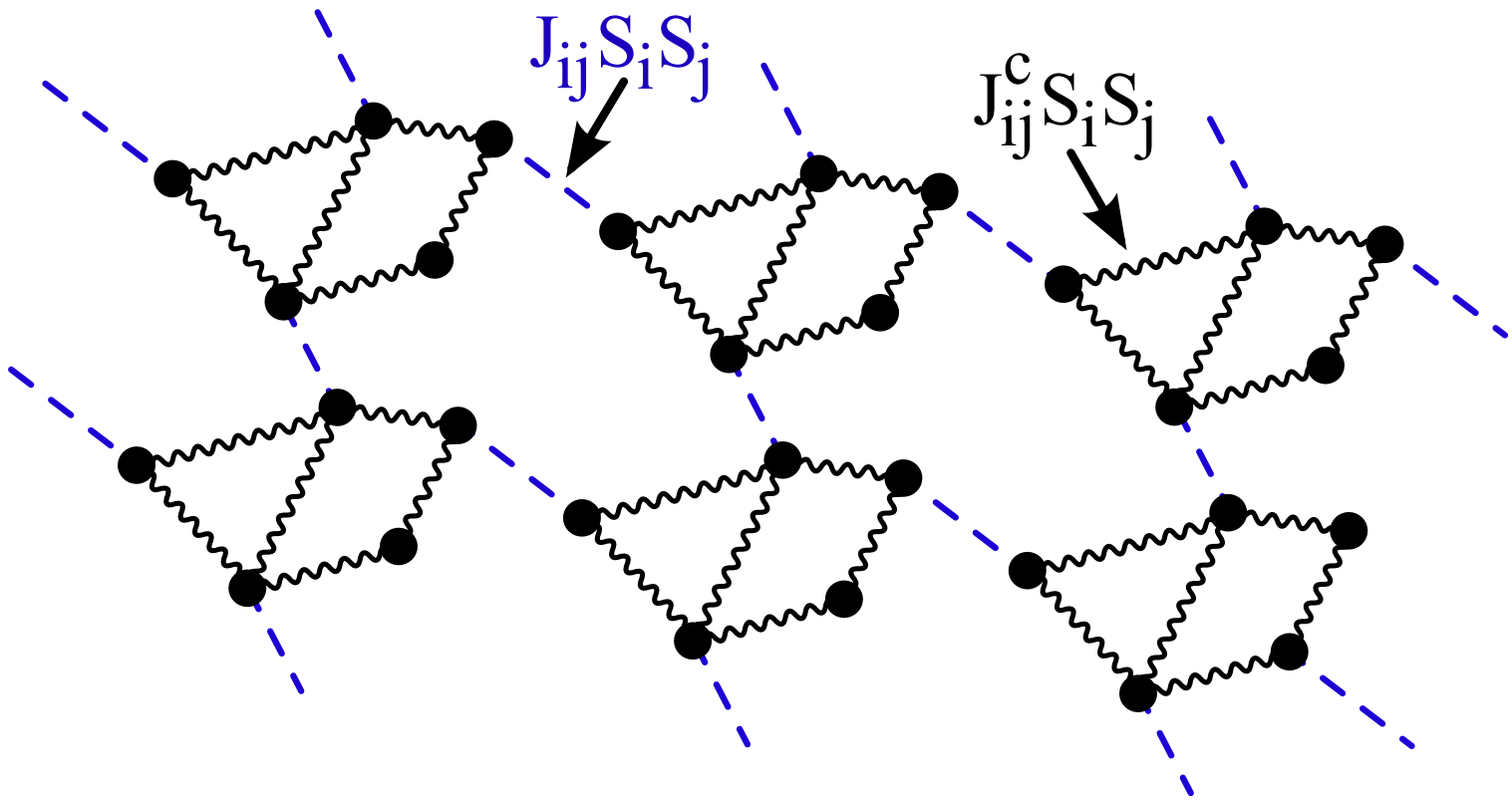
Peter Wölfle
Karlsruhe

Christian Platt
Würzburg

JR and Ronny Thomale, Phys. Rev. B **89**, 024412 (2014)

- JR and P. Wölfle, Phys. Rev. B **81**, 144410 (2010)
- JR, R. Thomale, and S. Trebst, Phys. Rev. B **84**, 100406 (2011)
- Y. Singh, S. Manni, JR, T. Berlijn, R. Thomale, W. Ku, S. Trebst, and P. Gegenwart, Phys. Rev. Lett. **108**, 127203 (2012)
- JR, R. Thomale, S. Rachel, arXiv:1404.5818 (2014)

Cluster spin models



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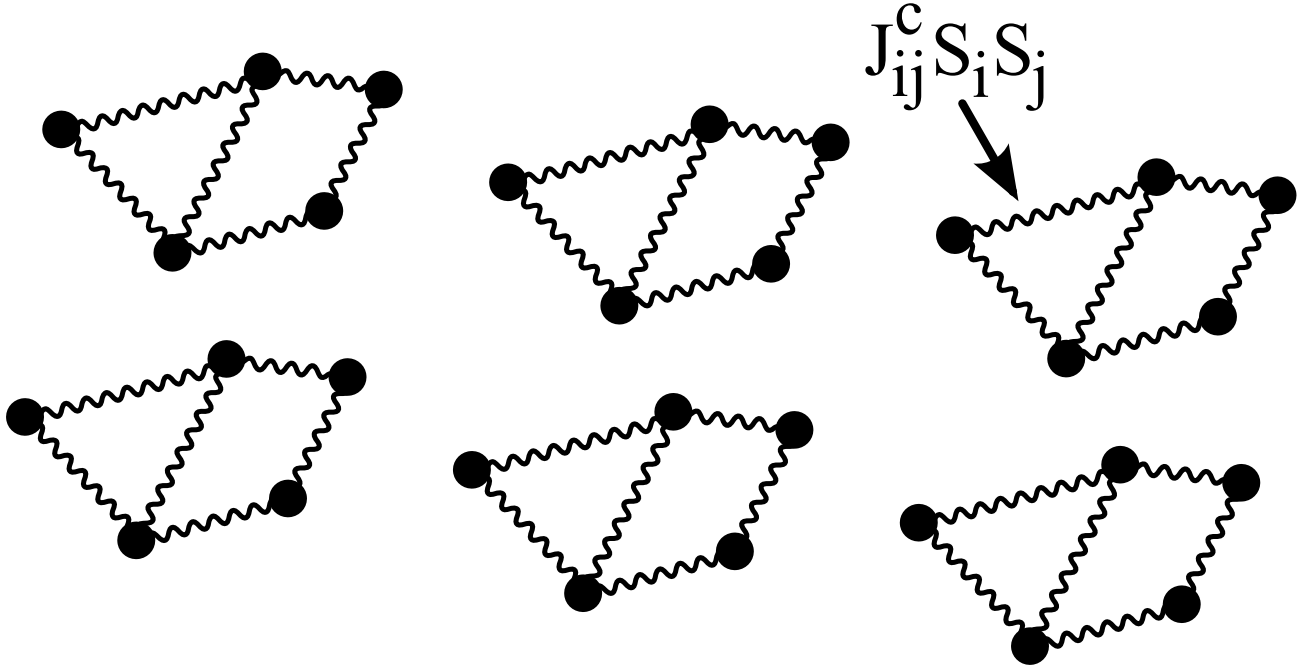
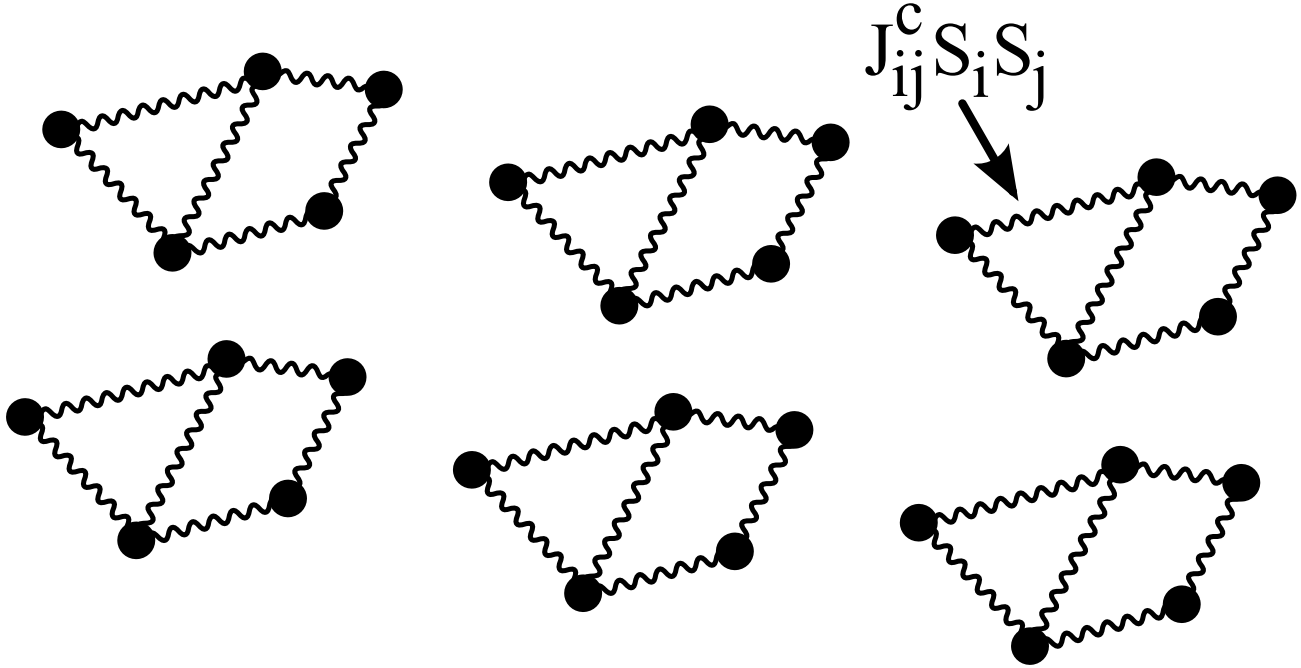
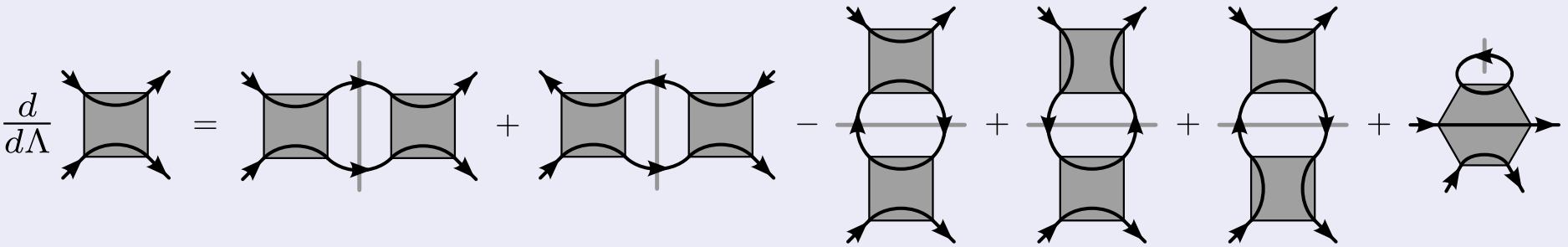


Cluster spin models



Use functional renomoralization-group method:



Outline

Pseudofermion FRG

Pseudo fermions

Introduce two fermionic operators $f_{i\uparrow}$, $f_{i\downarrow}$ for each lattice site i. Then:

$$S_i^\mu = \frac{1}{2} f_i^\dagger \sigma^\mu f_i \quad \text{with} \quad f_i = \begin{pmatrix} f_{i\uparrow} \\ f_{i\downarrow} \end{pmatrix}$$

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Spin space is two-dimensional ($|\uparrow\rangle$, $|\downarrow\rangle$) while two fermions define a four-dimensional space ($|0,0\rangle$, $|0,1\rangle$, $|1,0\rangle$, $|1,1\rangle$).

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A spin 1/2 is only realized in the subspace with $f_{i\uparrow}^\dagger f_{i\uparrow} + f_{i\downarrow}^\dagger f_{i\downarrow} = 1$ (one fermion per site)!

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Empty and doubly occupied sites carry spin zero and act like vacancies in the lattice

$\Longrightarrow$ excitation energy of order J

$\Longrightarrow$ unphysical occupations are naturally suppressed at zero temperature

Fermionic Hamiltonian

$$H = \sum_{ij} J_{ij}\, \mathbf{S}_i \mathbf{S}_j \longrightarrow \frac{1}{4} \sum_{ij} \sum_{\mu} J_{ij} \left(f_i^\dagger \sigma^\mu f_i \right) \left(f_j^\dagger \sigma^\mu f_j \right)$$

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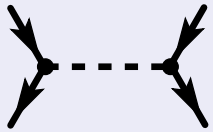
Diagrammatics in the fermions:

bare progagator: $G_0(i\omega) = \frac{1}{i\omega} =$ 

bare self energy: $\Sigma_0 = 0$

interaction vertex: $\Gamma_0 =$  $\sim J_{ij}$

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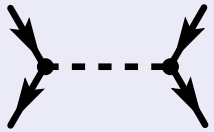
interaction vertex: $\Gamma_0 =$  $\sim J_{ij}$

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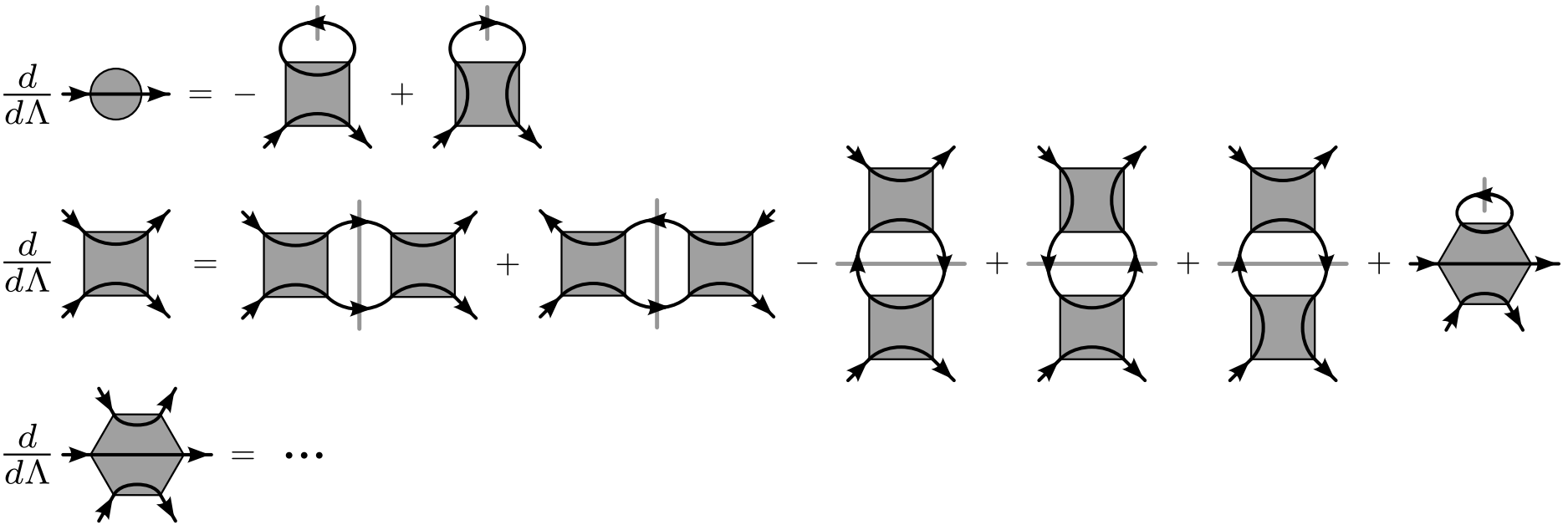
FRG may be applied (relatively) straightforwardly:
Introduce infrared frequency cutoff in the propagator:

$$G_0(i\omega) = \frac{1}{i\omega} \quad \longrightarrow \quad G_0^\Lambda(i\omega) = \frac{\Theta(|\omega| - \Lambda)}{i\omega}$$

Pseudofermion FRG

Define a flowing self energy Σ^Λ and a two-particle vertex $\Gamma^\Lambda(1', 2'; 1, 2)$, "1" $= \{\omega_1, i_1, \alpha_1\}$. $\Longrightarrow$ **FRG equations:**



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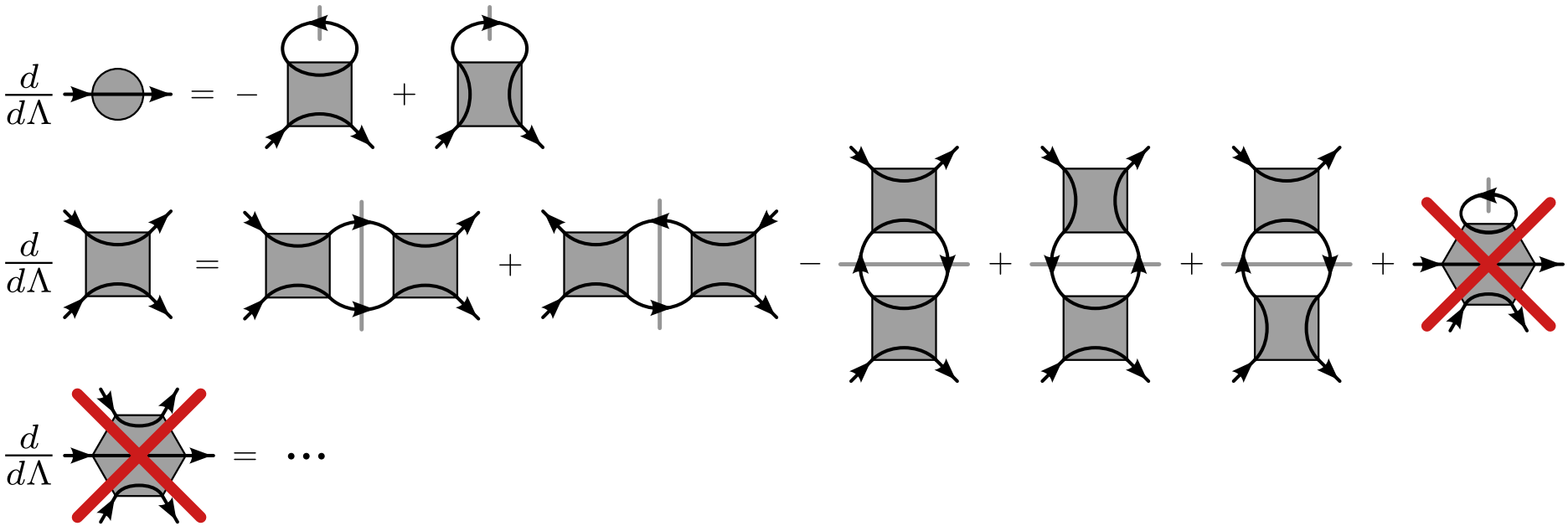

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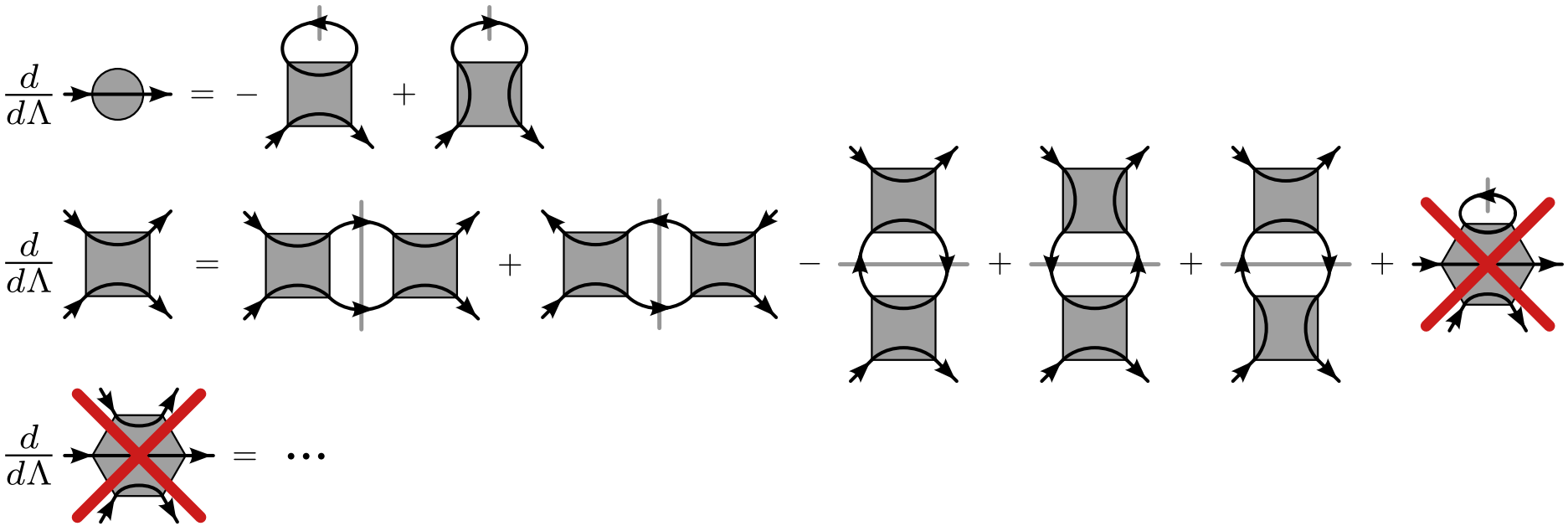

Initial conditions:

$\Sigma^{\Lambda\to\infty} = 0$

$\Gamma^{\Lambda\to\infty}(1', 2'; 1, 2) = \frac{1}{4} J_{i_1, i_2} \sigma^{\mu}_{\alpha_{1'}\alpha_1} \sigma^{\mu}_{\alpha_{2'}\alpha_2} \delta_{i_{1'} i_1} \delta_{i_{2'} i_2} - (i_1 \leftrightarrow i_2, \alpha_1 \leftrightarrow \alpha_2)$

Pseudofermion FRG

✓ This type of FRG approach works surprisingly well for 2D spin models

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✗ there is no well defined point of expansion (however, certain mean-field limits describing magnetic order and disorder are included exactly).

✗ 0D spin clusters may not be treated accurately.

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Can this be resolved within an cluster FRG approach which:

✓ uses the isolated cluster limit as well defined expansion point?

✓ treats finite spin clusters exactly?

Cluster implementation

See also:

A. Rançon and N. Dupuis, Phys. Rev. B 83, 172501 (2011)

A. Rançon and N. Dupuis, Phys. Rev. B 84, 174513 (2011)

M. Kinza, J. Ortloff, J. Bauer, and C. Honerkamp, Phys. Rev. B 87, 035111 (2013)

C. Taranto, S. Andergassen, J. Bauer, K. Held, A. Katanin, W. Metzner, G. Rohringer, and A. Toschi, Phys. Rev. Lett. 112, 196402 (2014)

→ Talk by A. Toschi, 17:50 Session VIII

Exact cluster vertices

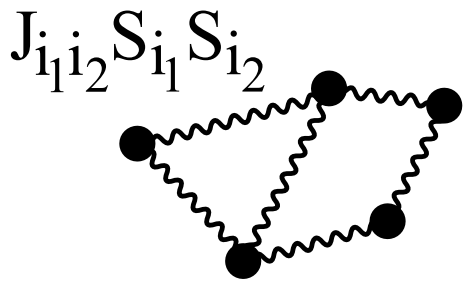
General idea: Replace

$$\Gamma^{\Lambda\to\infty}(1',2';1,2) = \frac{1}{4} J_{i_1,i_2} \sigma^{\mu}_{\alpha_{1'}\alpha_1} \sigma^{\mu}_{\alpha_{2'}\alpha_2} \delta_{i_{1'}i_1} \delta_{i_{2'}i_2} - (i_1 \leftrightarrow i_2, \alpha_1 \leftrightarrow \alpha_2)$$

in the initial conditions by the exact cluster vertex $\Gamma^{\text{ex}}(1',2';1,2)$

if J_{i_1,i_2} is a coupling within a cluster.

Then the isolated clusters are treated exactly!



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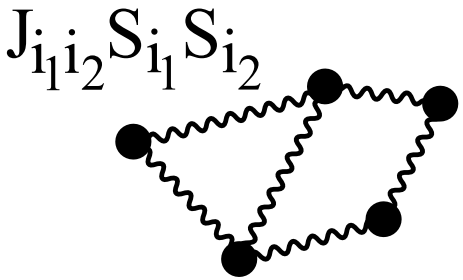
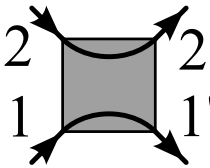


Is this allowed? Which consequences does it have on the FRG scheme?

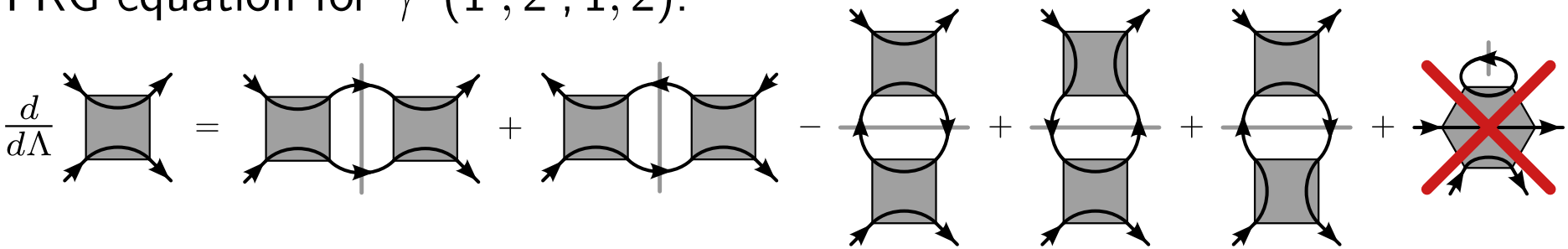
One severe difficulty indeed arises:

FRG equations

First parametrize: $\Gamma^\Lambda(1',2';1,2) = \gamma^\Lambda(1',2';1,2) - \gamma^\Lambda(1',2';2,1)$ with

$\gamma^\Lambda(1',2';1,2) = \gamma^\Lambda(2',1';2,1)$ and $\gamma^\Lambda(1',2';1,2) =$  $\sim \delta_{i_{1'} i_1} \delta_{i_{2'} i_2}$

FRG equation for $\gamma^\Lambda(1',2';1,2)$:



$$\frac{\partial}{\partial\Lambda}\gamma^\Lambda(1',2';1,2) = \frac{1}{2\pi}\sum_{3,4}\big[\gamma^\Lambda(1',2';3,4)\gamma^\Lambda(3,4;1,2)$$
$$+\gamma^\Lambda(2',4;3,1)\gamma^\Lambda(3,1';2,4) - \gamma^\Lambda(1',4;1,3)\gamma^\Lambda(3,2';4,2)$$
$$+\gamma^\Lambda(1',4;1,3)\gamma^\Lambda(3,2';2,4) + \gamma^\Lambda(1',4;3,1)\gamma^\Lambda(3,2';4,2)\big]$$
$$\times\left(G^\Lambda(i\omega_3)S^\Lambda(i\omega_4) + G^\Lambda(i\omega_4)S^\Lambda(i\omega_3)\right)$$

single scale propagator $S^\Lambda = G^\Lambda[\partial_\Lambda (G_0^\Lambda)^{-1}]G^\Lambda$

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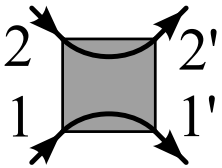
$\gamma^\Lambda(1',2';1,2) = \gamma^\Lambda(2',1';2,1)$ and $\gamma^\Lambda(1',2';1,2) =$ 

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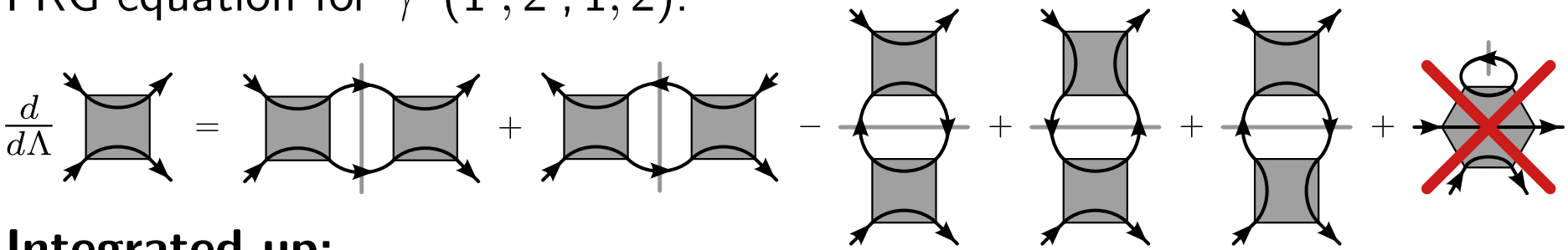

Integrated up:

$$\gamma^\Lambda(1',2';1,2) = \gamma^\infty(1',2';1,2) + \int_\infty^\Lambda d\Lambda' \frac{1}{2\pi} \sum_{3,4}$$
$$\times \big[\gamma^{\Lambda'}(1',2';3,4)\gamma^{\Lambda'}(3,4;1,2) + \gamma^{\Lambda'}(2',4;3,1)\gamma^{\Lambda'}(3,1';2,4)$$
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with $P^\Lambda(i\omega_3, i\omega_4) = G^\Lambda(i\omega_3)S^\Lambda(i\omega_4) + G^\Lambda(i\omega_4)S^\Lambda(i\omega_3)$

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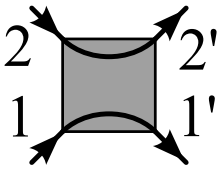
$\gamma^\Lambda(1',2';1,2) = \gamma^\Lambda(2',1';2,1)$ and $\gamma^\Lambda(1',2';1,2) =$ 

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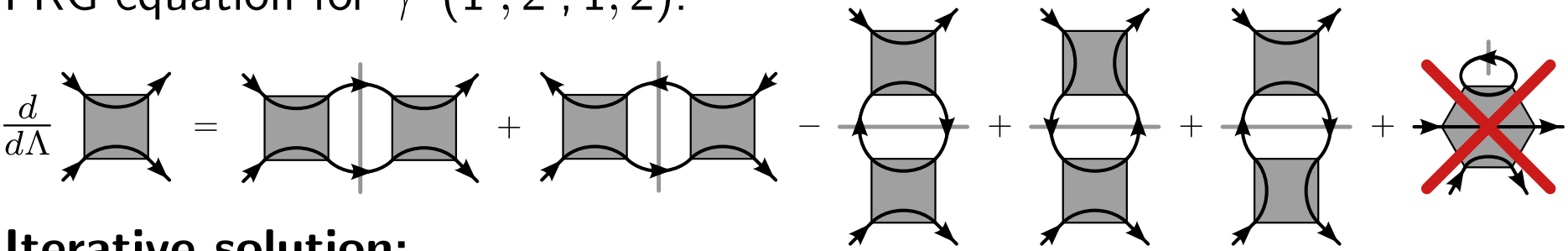

Iterative solution:

Set $\gamma_0 = \gamma^\infty$ and insert the solutions successively, yielding γ_1, γ_2,...

$$\gamma^\Lambda_{n+1}(1',2';1,2) = \gamma^\infty(1',2';1,2) + \int_\infty^\Lambda d\Lambda' \frac{1}{2\pi} \sum_{3,4}$$
$$\times \Big[\gamma_n^{\Lambda'}(1',2';3,4)\gamma_n^{\Lambda'}(3,4;1,2) + \gamma_n^{\Lambda'}(2',4;3,1)\gamma_n^{\Lambda'}(3,1';2,4)$$
$$- \gamma_n^{\Lambda'}(1',4;1,3)\gamma_n^{\Lambda'}(3,2';4,2) + \gamma_n^{\Lambda'}(1',4;1,3)\gamma_n^{\Lambda'}(3,2';2,4)$$
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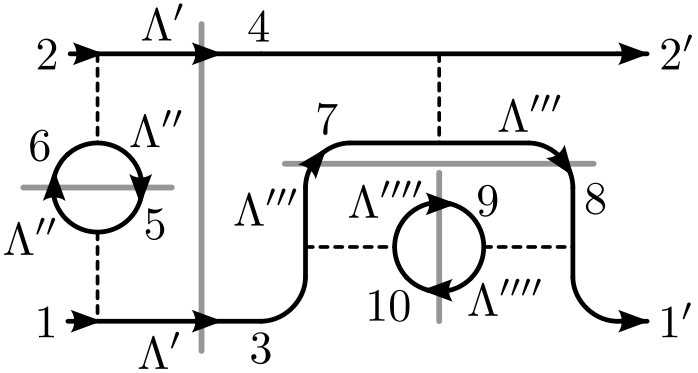
Example for a diagrammatic contribution to $\gamma_3^{\Lambda}(1',2';1,2)$:



$$= \int_{\infty}^{\Lambda} d\Lambda' \int_{\infty}^{\Lambda'} d\Lambda'' \int_{\infty}^{\Lambda'} d\Lambda''' \int_{\infty}^{\Lambda'''} d\Lambda'''' \frac{1}{(2\pi)^4} \sum_{3\cdots 10}$$

$$\times \gamma^{\infty}(3,6;1,5)\gamma^{\infty}(5,4;6,2)\gamma^{\infty}(8,2';7,4)$$

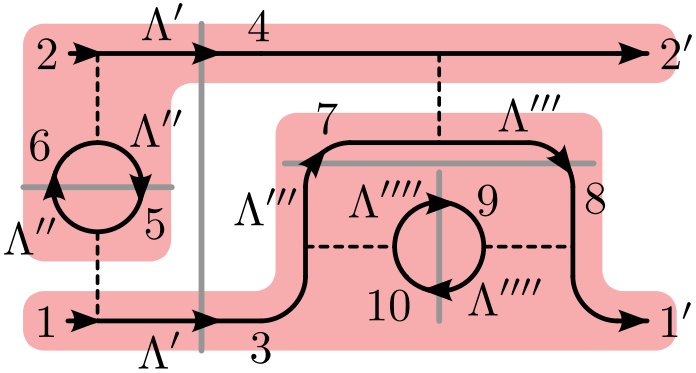
$$\times \gamma^{\infty}(9,7;10,3)\gamma^{\infty}(1',10;8,9)$$

$$\times P^{\Lambda'}(i\omega_3,i\omega_4)P^{\Lambda''}(i\omega_5,i\omega_6)P^{\Lambda'''}(i\omega_7,i\omega_8)P^{\Lambda''''}(i\omega_9,i\omega_{10})$$

Iterative solution

Example for a diagrammatic contribution to $\gamma_3^{\Lambda}(1',2';1,2)$:

Assume that the propagator lines (sites) 4,5,6 and 3,7,8,9,10 are located on the same cluster, respectively.



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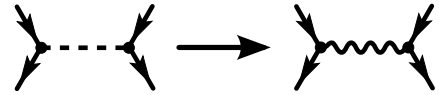
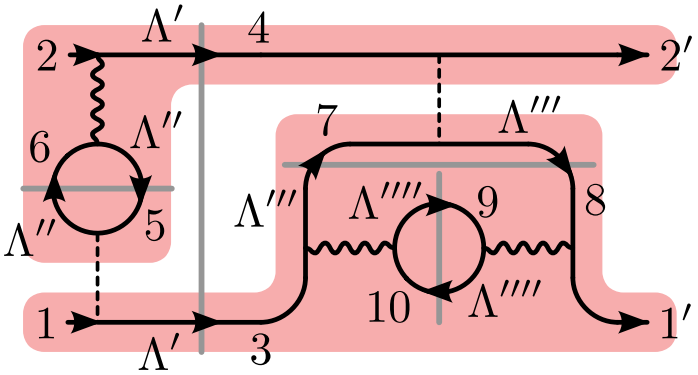
Using the new initial conditions, the bare interaction needs to be replaced by the exact cluster vertex for all intra-cluster couplings,  .



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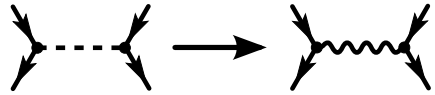
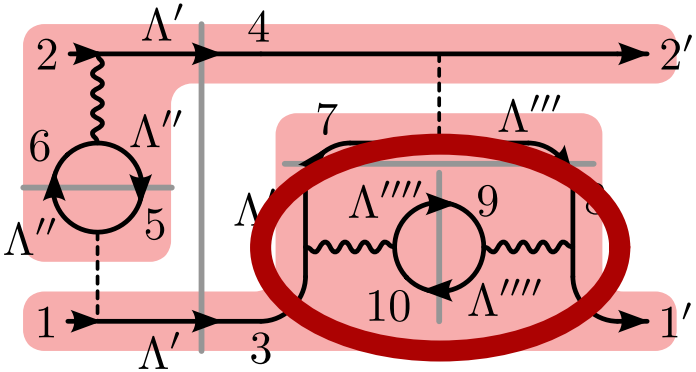
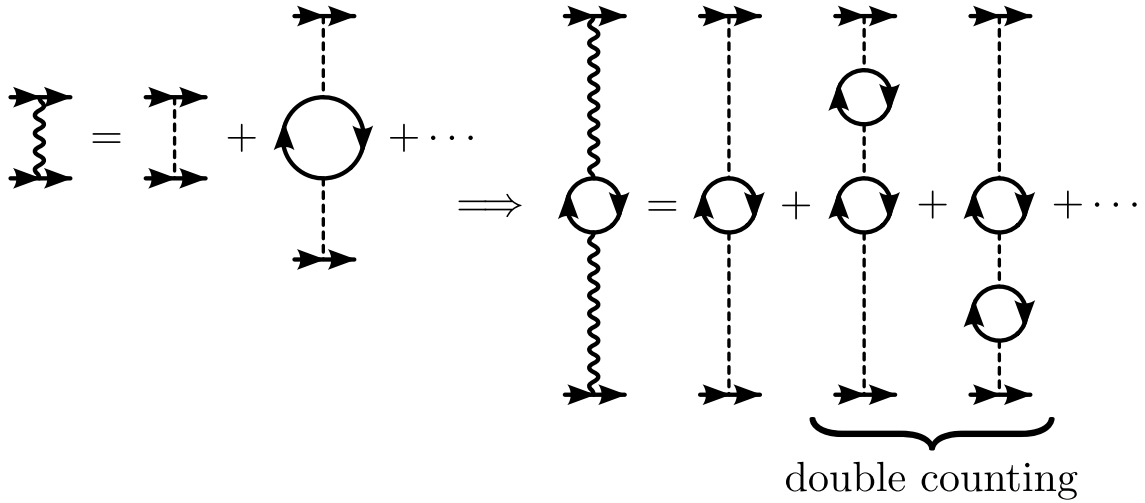
Using the new initial conditions, the bare interaction needs to be replaced by the exact cluster vertex for all intra-cluster couplings,  .



$$= \int_{\infty}^{\Lambda} d\Lambda' \int_{\infty}^{\Lambda'} d\Lambda'' \int_{\infty}^{\Lambda'} d\Lambda''' \int_{\infty}^{\Lambda'''} d\Lambda'''' \frac{1}{(2\pi)^4} \sum_{3\cdots 10}$$
$$\times \gamma^{\infty}(3,6;1,5)\gamma^{\infty}(5,4;6,2)\gamma^{\infty}(8,2';7,4)$$
$$\times \gamma^{\infty}(9,7;10,3)\gamma^{\infty}(1',10;8,9)$$
$$\times P^{\Lambda'}(i\omega_3, i\omega_4)P^{\Lambda''}(i\omega_5, i\omega_6)P^{\Lambda'''}(i\omega_7, i\omega_8)P^{\Lambda''''}(i\omega_9, i\omega_{10})$$

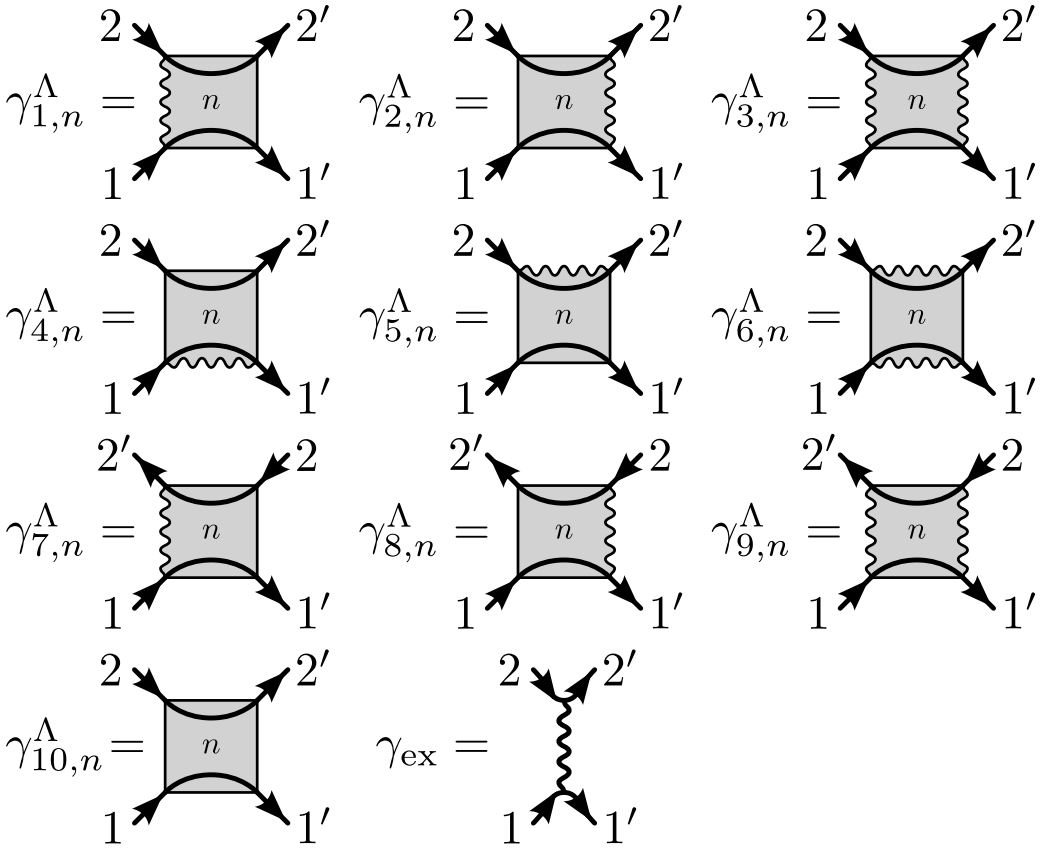
Over-counting of sub diagrams!

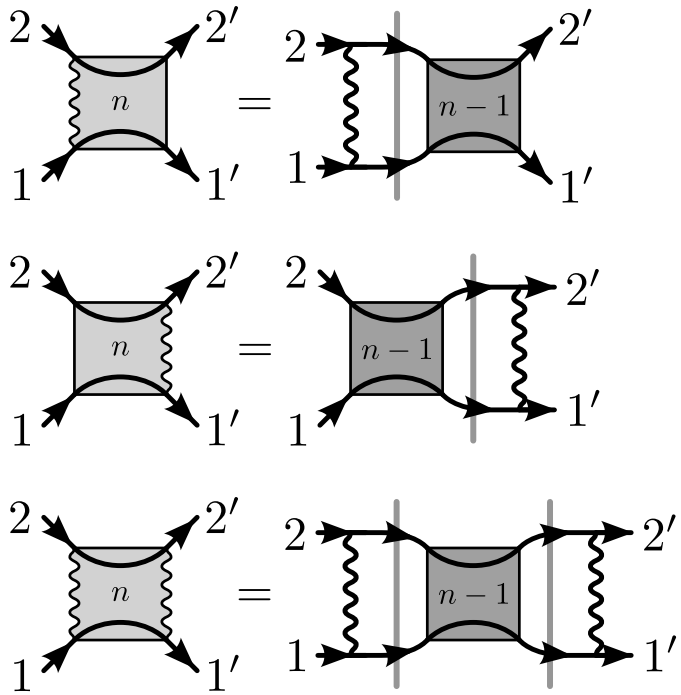


New classes of vertices

How can this over-counting of terms be avoided?

Define classes of vertices $\gamma^{\Lambda}_{1,n}$, $\gamma^{\Lambda}_{2,n}$, ..., $\gamma^{\Lambda}_{10,n}$ with $\gamma^{\Lambda}_{n} = \sum_{x=1}^{10} \gamma^{\Lambda}_{x,n} + \gamma^{\text{ex}}$

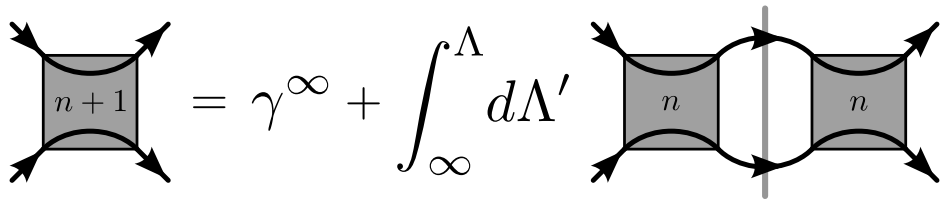




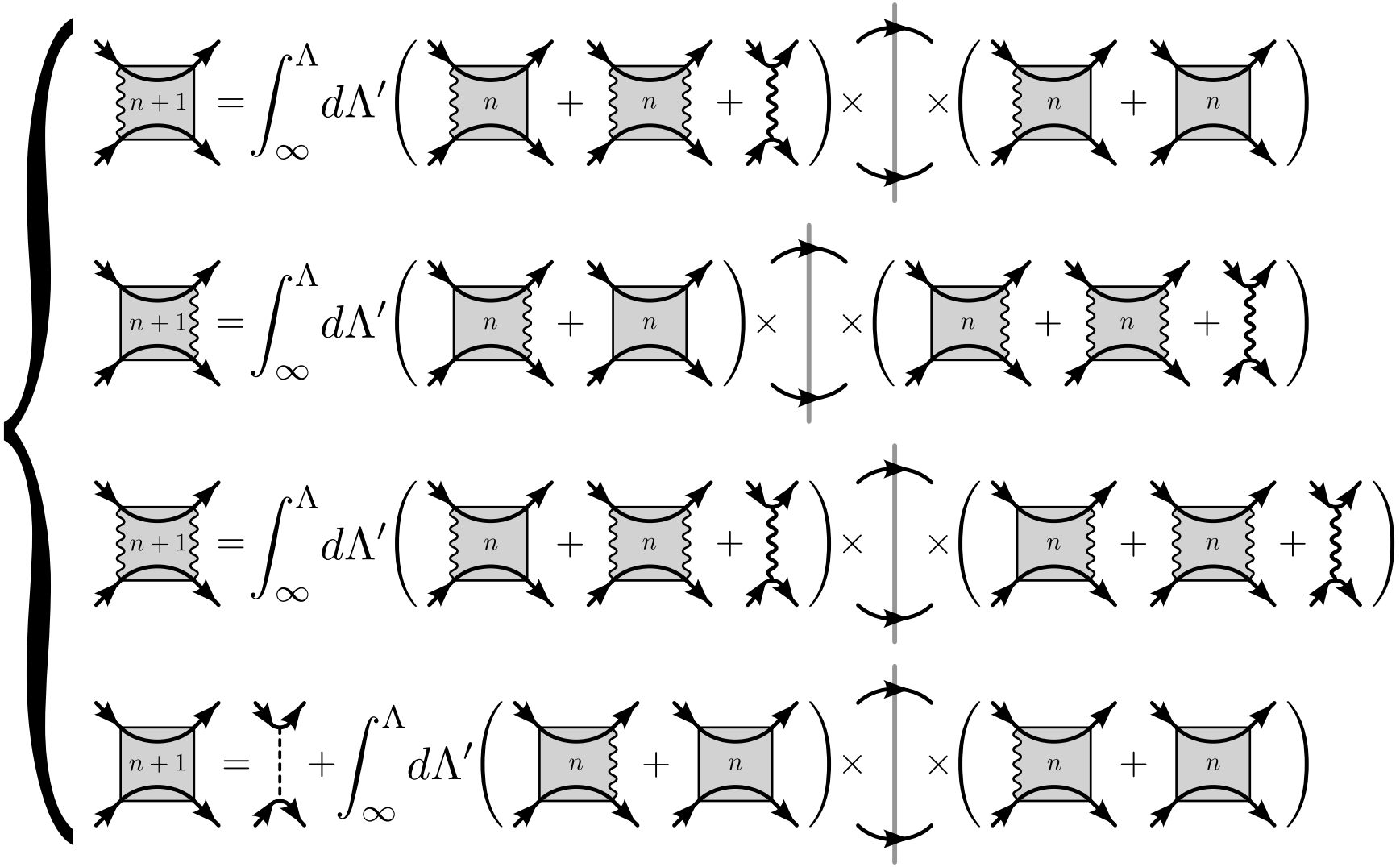
New classes of vertices

Express the FRG flow equations in terms of these new classes.

Example: particle-particle channel

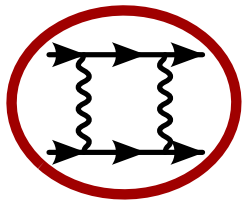


$\Rightarrow$

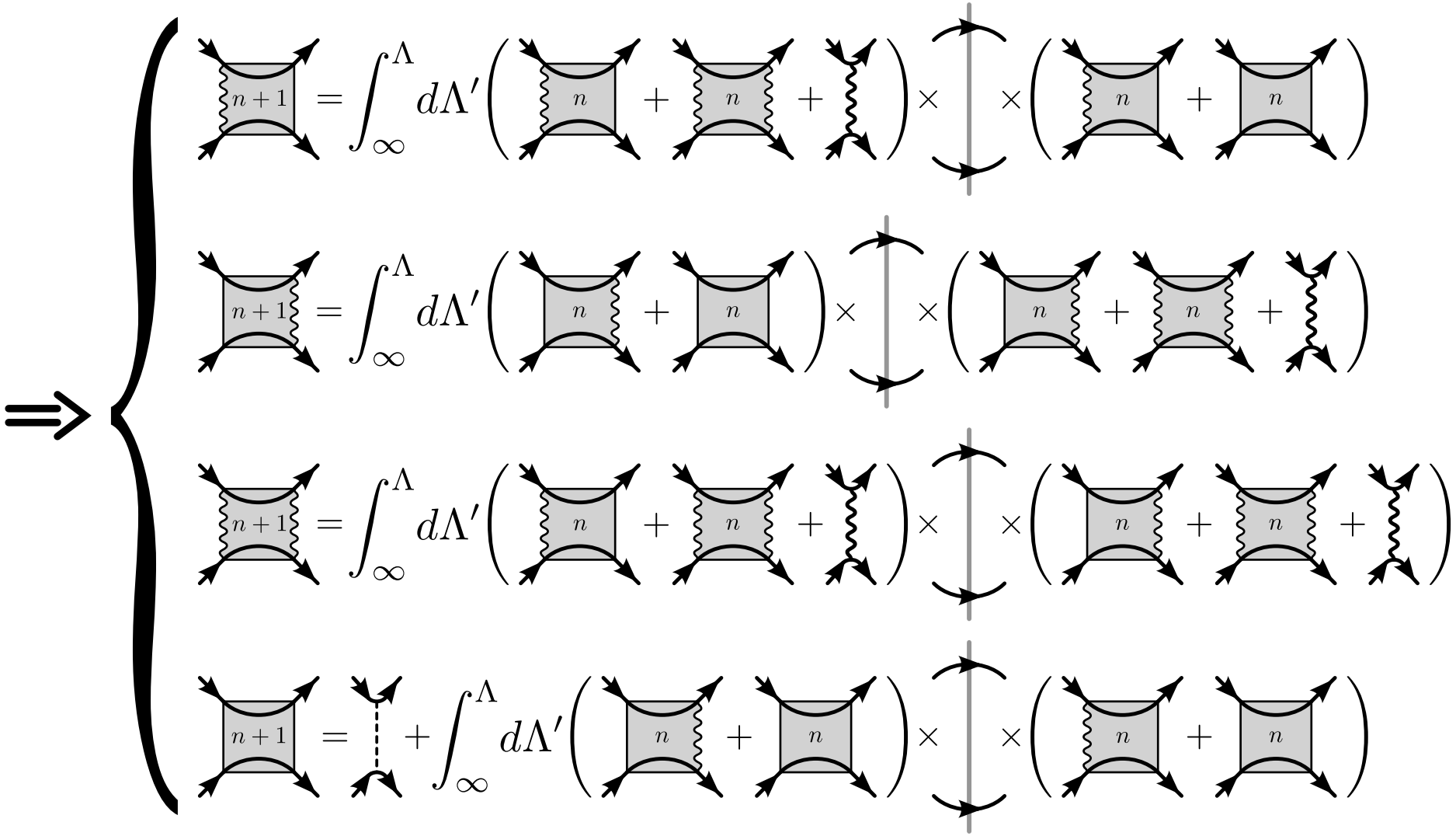


New classes of vertices

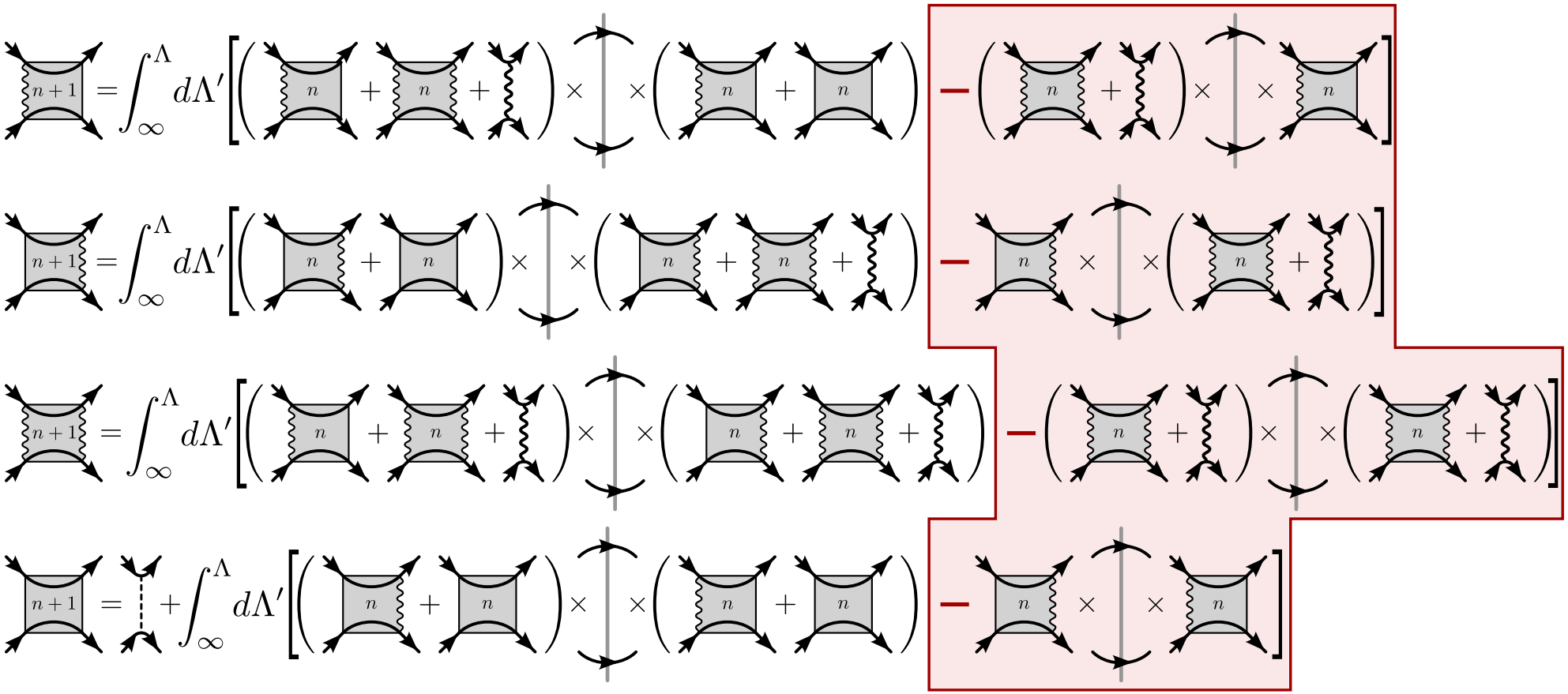
Express the FRG flow equations in terms of these new classes.



Example: particle-particle channel



Introduce counter terms

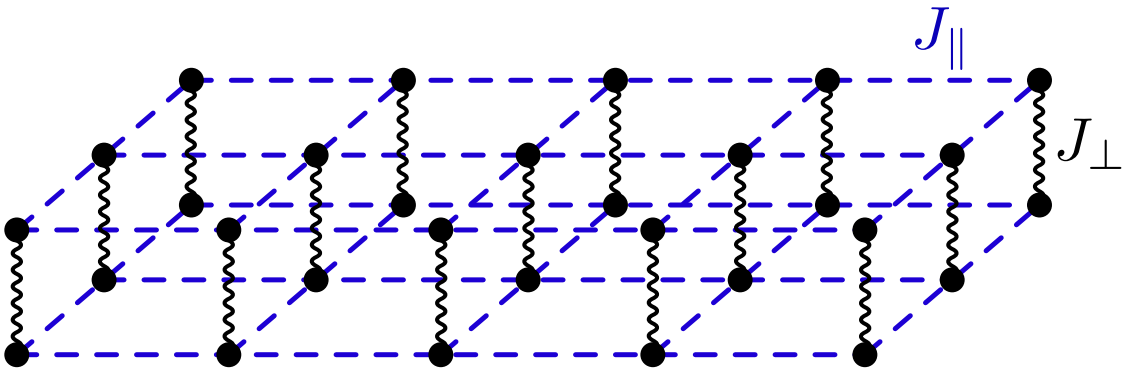


Counter terms cancel the redundant diagrams in each iteration step separately! (works similarly for the other interaction channels)

$\Longrightarrow$ Well defined cluster-expansion scheme.

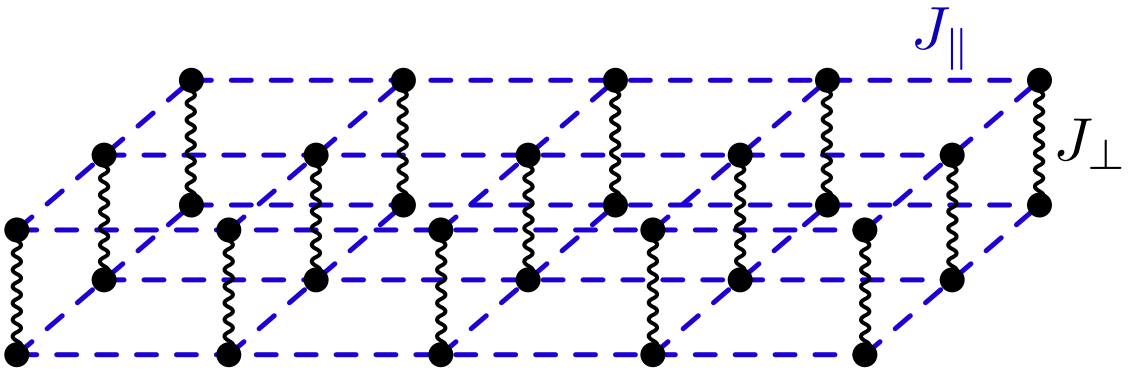
Application to the bilayer Heisenberg model

Bilayer Heisenberg model



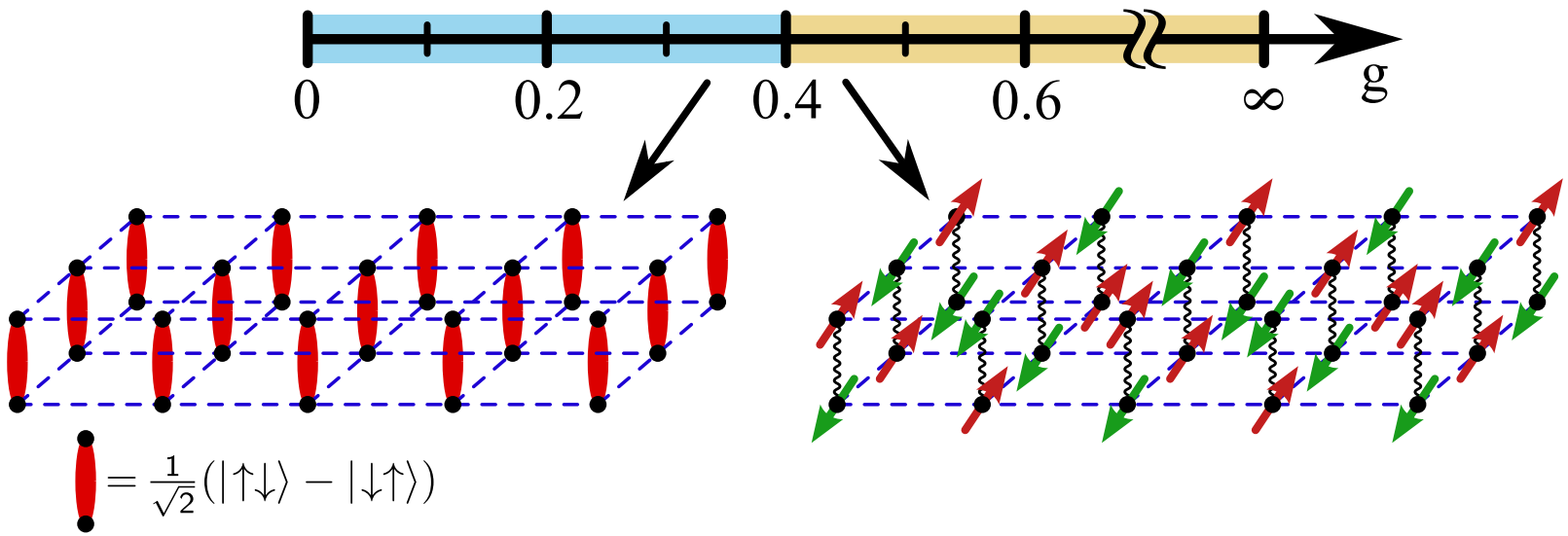
$$H = J_\parallel \sum_{\langle ij \rangle} \sum_{a=1,2} \mathbf{S}_{ia}\mathbf{S}_{ja} + J_\perp \sum_i \mathbf{S}_{i1}\mathbf{S}_{i2}$$

Bilayer Heisenberg model



$$H = J_\parallel \sum_{\langle ij \rangle} \sum_{a=1,2} \mathbf{S}_{ia}\mathbf{S}_{ja} + J_\perp \sum_i \mathbf{S}_{i1}\mathbf{S}_{i2}$$

Phase diagram for $J_\parallel$, $J_\perp > 0$ and $g = J_\parallel / J_\perp$:

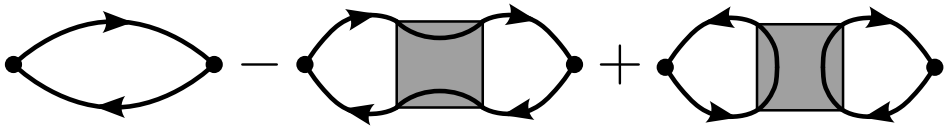


Numerical value from Monte Carlo: $g_c = 0.3965$

L. Wang, K. S. D. Beach, and A. W. Sandvik, Phys. Rev. B 73, 014431 (2006)

Bilayer Heisenberg model

Calculate the frequency dependent susceptibility via

$\chi^{\Lambda=0}(\mathbf{k},\omega) =$ 

$\mathbf{k} = (k_x, k_y, k_z)$ with $k_x, k_y \in [-\pi, \pi]$ and $k_z = 0, \pi$.

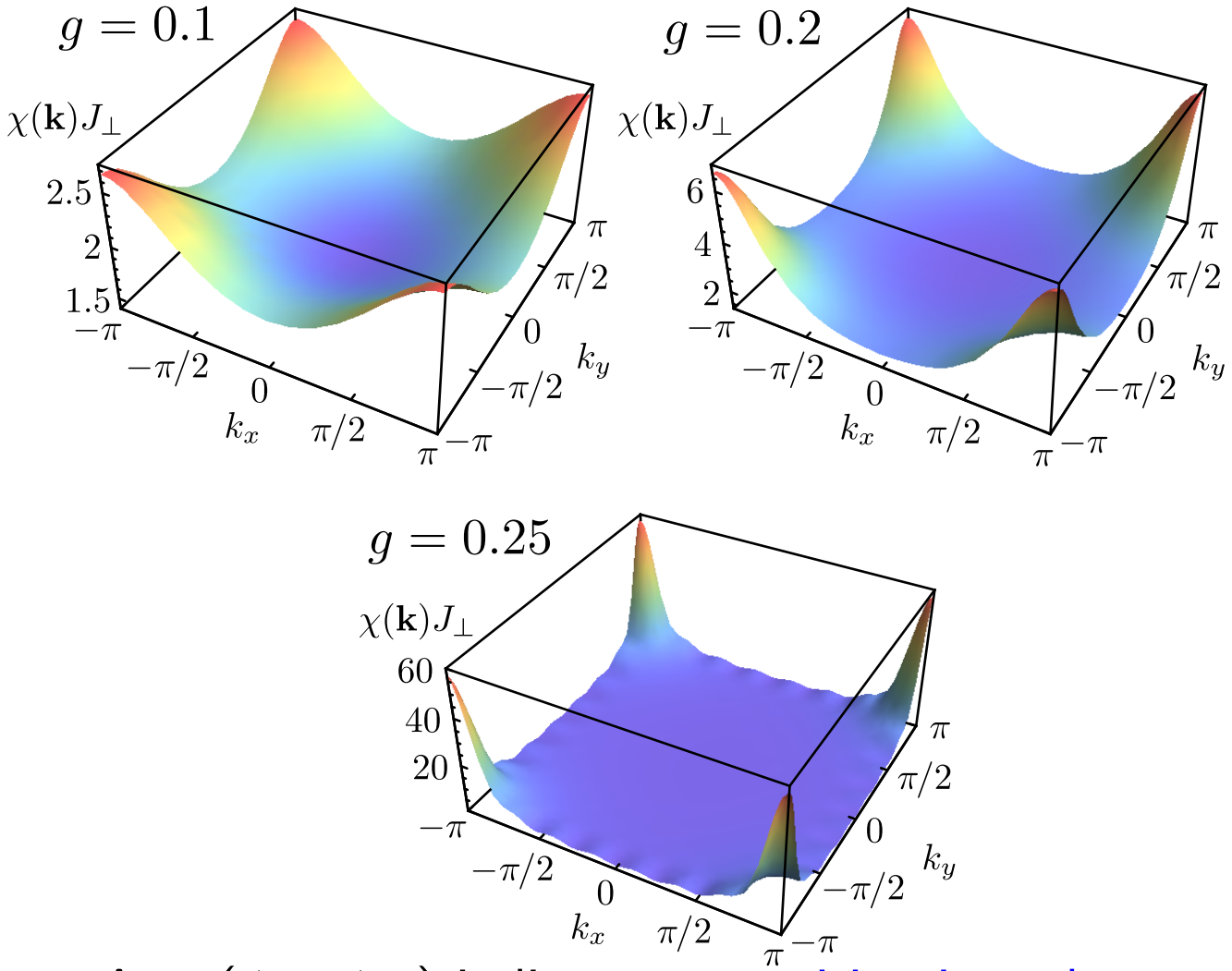
In the following $k_z = \pi$.

For a stable numerical implementation of the cluster FRG, some approximations and modifications are necessary.

(for details, see JR and Ronny Thomale, Phys. Rev. B **89**, 024412 (2014))

Bilayer Heisenberg model

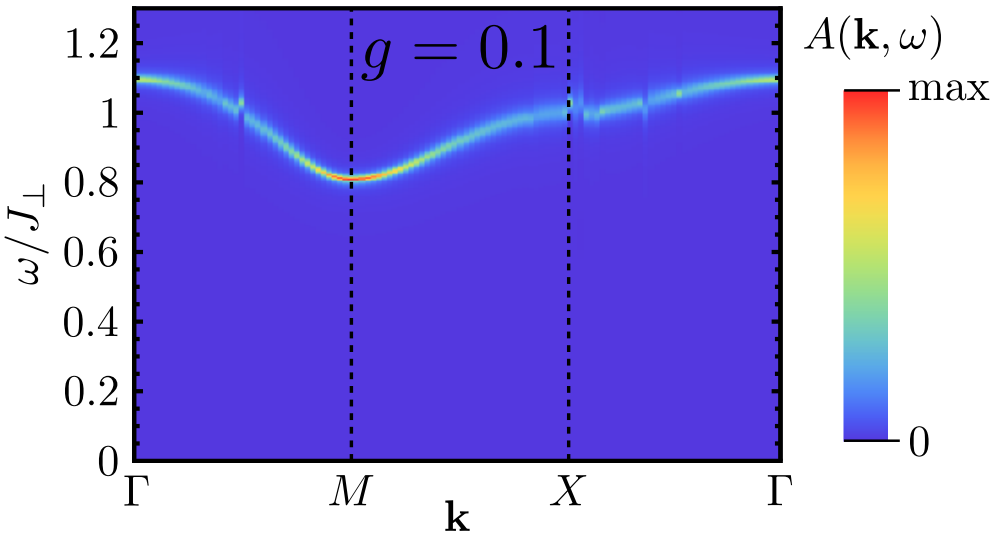
Results for the static susceptibility $\chi(\mathbf{k}) = \chi(\mathbf{k}, \omega = 0)$:

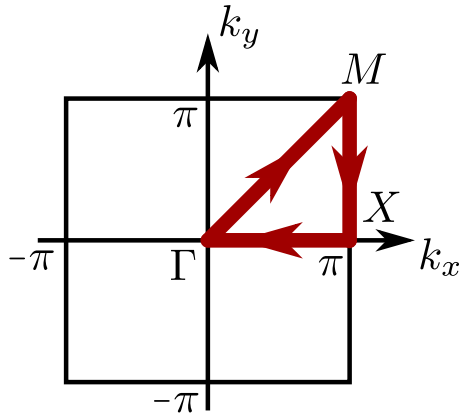


Sharp peaks at $\mathbf{k} = (\pm\pi, \pm\pi)$ indicate a transition into the antiferromagnetic Néel phase at $g \approx 0.27$.

Bilayer Heisenberg model

Calculate the spin-excitation spectrum $A(\mathbf{k},\omega) = \frac{1}{\pi}\mathrm{Im}\,\chi(\mathbf{k},\omega + i0^+)$ via analytical continuation (Padé approximation):





Bilayer Heisenberg model

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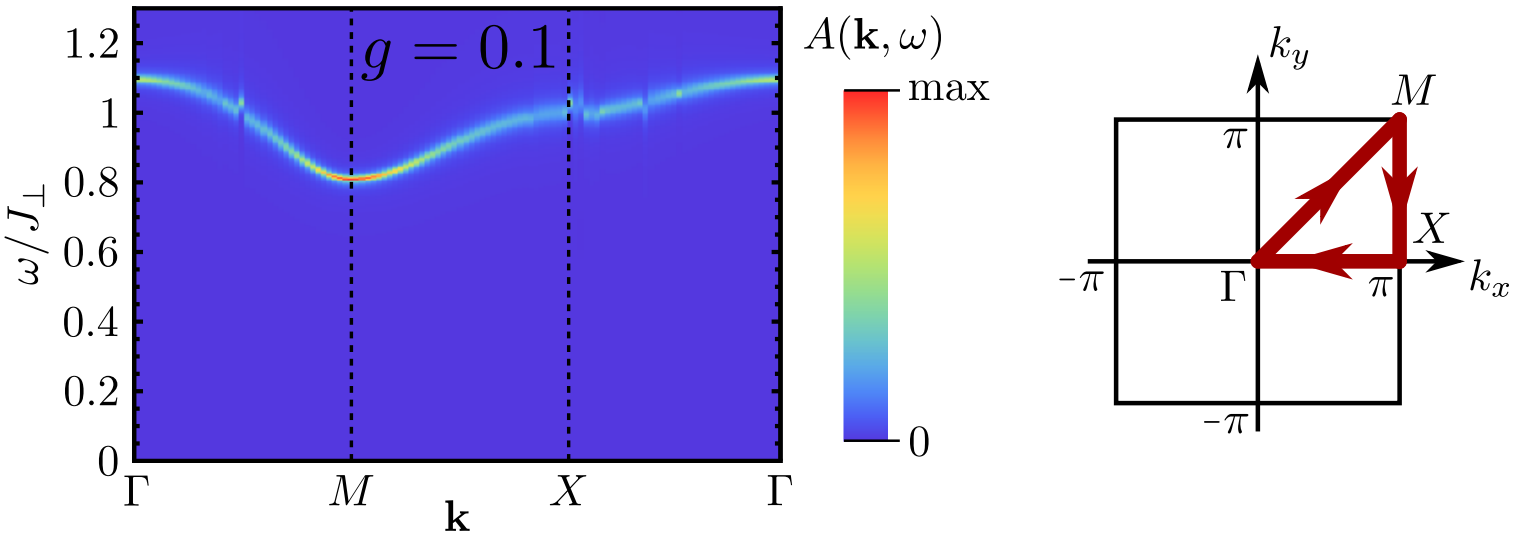


Fit a bosonic Green's function with a single excitation to $\chi(\mathbf{k},\omega)$

$$\chi(\mathbf{k},z) = W_{\mathbf{k}}\left(\frac{1}{z+E_{\mathbf{k}}+i\delta_{\mathbf{k}}} - \frac{1}{z-E_{\mathbf{k}}+i\delta_{\mathbf{k}}}\right)$$

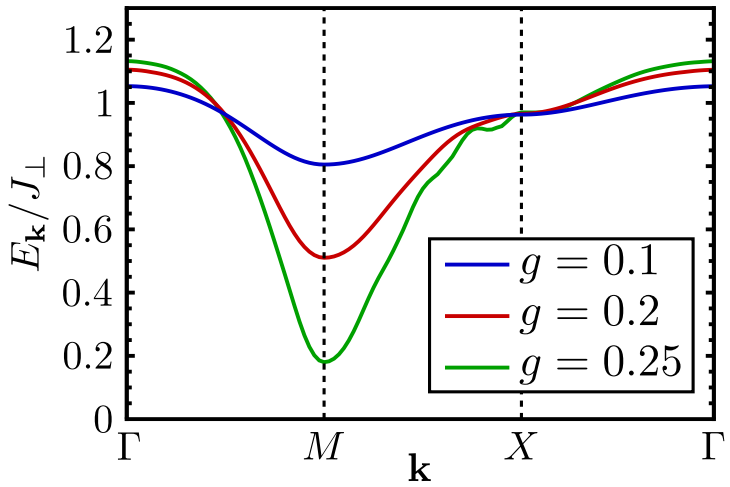
to obtain

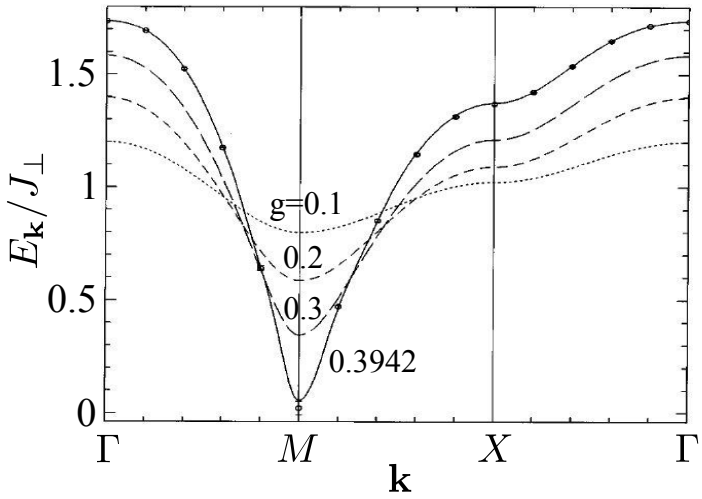
- the dispersion of spin excitations $E_{\mathbf{k}}$
- the quasiparticle weight $W_{\mathbf{k}}$
- the damping (inverse lifetime) $\delta_{\mathbf{k}}$

Bilayer Heisenberg model

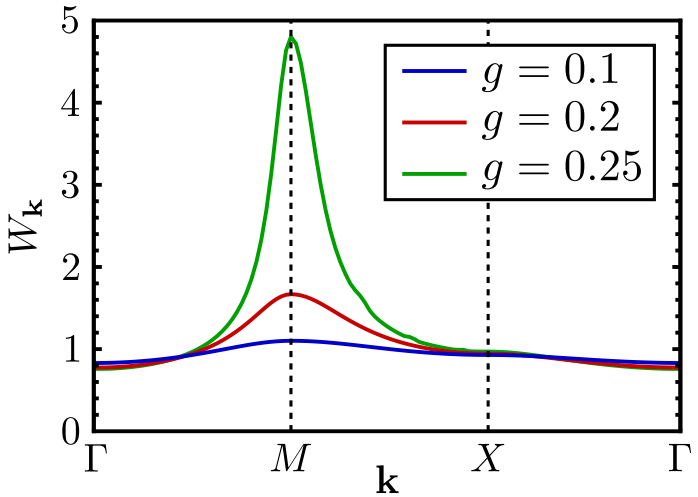
Dispersion $E_{\mathbf{k}}$ in comparison to dimer expansion:

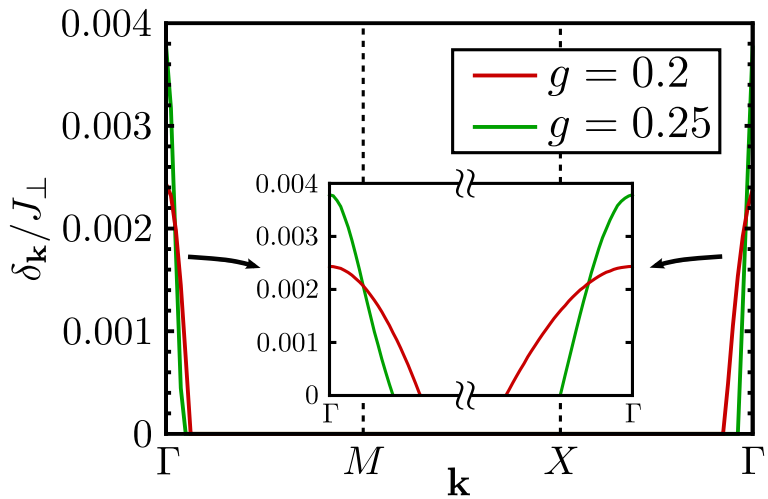
(Z. Weihong, Phys. Rev. B 55, 12267 (1997))





Quasiparticle weight $W_{\mathbf{k}}$ and damping $\delta_{\mathbf{k}}$:





Conclusion

Conclusion

- Within a cluster FRG approach the spin clusters are treated exactly while the inter-cluster couplings are addressed via RG.
- In order to circumvent an over-counting of diagrams, counter terms need to be introduced.
- A simplified numerical implementation yields qualitatively correct results for the bilayer Heisenberg model. (Improvements concerning g_c are possible.)
- The exact cluster vertices enter the initial conditions and only need to be evaluated once
  $\Longrightarrow$ Large spin clusters are possible (as long as the exact cluster vertices can be calculated)!

Thank you for your attention!