Phase diagram of the J_1-J_2 quantum Heisenberg model for arbitrary spin

Andreas Rückriegel

Institut für Theoretische Physik, Universität Frankfurt

ERG 2024, Les Diablerets,
September 25, 2024

A. Rückriegel, D. Tarasevych, and P. Kopietz,
Phys. Rev. B **109**, 184410 (2024)

Frustrated quantum spin systems

- Frustration: Major challenge for theoretical physics.
- Quantum fluctuations dominant for $T \to 0$.
  - $\Rightarrow$ Exotic ground states without classical long-range order.
- Paradigmatic model system: J_1-J_2 quantum Heisenberg antiferromagnet on the square lattice,

$$\mathcal{H} = J_1 \sum_{\langle ij \rangle_1} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + J_2 \sum_{\langle ij \rangle_2} \boldsymbol{S}_i \cdot \boldsymbol{S}_j \ .$$

- Consensus on phase diagram for $S = 1/2$:
  - Néel order for $J_2 \lesssim 0.4 J_1$, ordering wave vector $\boldsymbol{Q} = (\pi, \pi)$.
  - Stripe order for $J_2 \gtrsim 0.65 J_1$, with $\boldsymbol{Q} = (\pi, 0)$ or $\boldsymbol{Q} = (0, \pi)$.
  - Quantum paramagnet in the intermediate, strongly frustrated regime.
- For $S > 1/2$: Reduced quantum fluctuations should reduce paramagnetic regime, which vanishes for $S \to \infty$.

Spin functional renormalization group

Spin FRG approach: Continuously deform exchange couplings

$$J(\boldsymbol{k}) \rightarrow J_\Lambda(\boldsymbol{k})\ , \quad \Lambda \in [0,1]\ ,$$

such that

1. $J_{\Lambda=0}(\boldsymbol{k}) = 0$ (isolated spins),
2. $J_{\Lambda=1}(\boldsymbol{k}) = J(\boldsymbol{k})$ (full interacting system).

$\Rightarrow$ Exact flow equation for the Λ-dependent generating functional of imaginary-time-ordered spin correlation functions.

- Advantages of the spin functional renormalization group:
  - Bosonic Wetterich equation for irreducible spin vertices.
  - Works directly with the physical spin degrees of freedom.
  - Arbitrary S without additional cost.
- Non-trivial initial conditions because of $SU(2)$ spin algebra.

[Krieg, Kopietz, Phys. Rev. B **99**, 060403(R) (2019)]

Initial conditions & spin conservation

- Local spin conservation $\partial_t \boldsymbol{S}_i = 0$ implies nonanalytic frequency dependence of the spin-spin correlation function at $\Lambda = 0$,

$$G_0(\omega) = \delta_{\omega,0} S(S+1)/3T \ .$$

⇒ Nonanalytic $\delta_{\omega,0}$ terms are inherited by all higher-order correlation functions through the hierarchy of equations of motion:

$$\omega_1 G_0^{xyz}(\omega_1, \omega_2, \omega_3) = G_0(\omega_2) - G_0(\omega_3) \ ,$$

$$\omega_1 G_0^{xxyy}(\omega_1, \ldots \omega_4) = -G_0^{xyz}(\omega_2, \omega_3, \omega_1 + \omega_4) - G_0^{xyz}(\omega_2, \omega_4, \omega_1 + \omega_3) \ ,$$

$$\vdots$$

⇒ Legendre transform of generating functional does not exist at $\Lambda = 0$.

- Solution: Treat dynamic and static fluctuations differently.

  [Goll, Tarasevych, Krieg, Kopietz, Phys. Rev. B **100**, 174424 (2019)]

Ergodicity & hybrid functional

- Interacting spins at $\Lambda > 0$:
  - Spin conservation only holds globally, $G_\Lambda(\boldsymbol{k} = 0, \omega \neq 0) = 0$.
  - Ergodicity: All static susceptibilities (Kubo, isothermal, adiabatic, ...) have to agree for $\boldsymbol{k} \neq 0$. [Chiba *et al.* PRL 2020]

  $\Rightarrow$ $G_\Lambda(\boldsymbol{k} \neq 0, \omega)$ expected to be continuous for $\omega \to 0$.

$\Rightarrow$ Parametrize dynamic spin susceptibility as

$$G_\Lambda(\boldsymbol{k}, \omega \neq 0) = \frac{\Pi_\Lambda(\boldsymbol{k}, \omega)}{1 + G_\Lambda^{-1}(\boldsymbol{k})\Pi_\Lambda(\boldsymbol{k}, \omega)} \, , \qquad \Pi_\Lambda(\boldsymbol{k} = 0, \omega \neq 0) = 0 \, ,$$

$$G_\Lambda(\boldsymbol{k}, \omega = 0) = G_\Lambda(\boldsymbol{k}) = \frac{1}{J_\Lambda(\boldsymbol{k}) + \Sigma_\Lambda(\boldsymbol{k})} \, , \quad \lim_{\omega \to 0} \Pi_\Lambda^{-1}(\boldsymbol{k} \neq 0, \omega) = 0 \, .$$

- Flow equations for $\Sigma_\Lambda(\boldsymbol{k})$ and $\Pi_\Lambda(\boldsymbol{k}, \omega \neq 0)$: Hybrid functional.
  - Statics: 1-line irreducible with respect to classical propagator $G_\Lambda(\boldsymbol{k})$.
  - Dynamics: 1-line irreducible with respect to $\tilde{J}_\Lambda(\boldsymbol{k}) = G_\Lambda^{-1}(\boldsymbol{k})$.

    [Tarasevych, Kopietz, Phys. Rev. B **104**, 024423 (2021)]

Temperature flow

Deformation scheme

$$J_\Lambda(\boldsymbol{k}) = \Lambda J(\boldsymbol{k}) = \bar{\Lambda} T J(\boldsymbol{k}) \quad \text{with} \quad \bar{\Lambda} \in [0, 1/T].$$

- Without external magnetic fields: Explicit T-dependence can be removed by rescaling frequencies and vertices,

$$\omega = \bar{\omega} T \,, \quad \Sigma_\Lambda(\boldsymbol{k}) = T \bar{\Sigma}(\boldsymbol{k}) \,, \quad \Pi_\Lambda(\boldsymbol{k}, \omega) = \bar{\Pi}_\Lambda(\boldsymbol{k}, \bar{\omega})/T \,, \ldots$$

$\Rightarrow$ Effectively T-independent problem at fixed $\bar{\Lambda}$.

$\Rightarrow$ T-dependence: Flow from $\bar{\Lambda} = 0$ $(T \to \infty)$ to $\bar{\Lambda} = 1/T$.

$\Rightarrow$ Flow perturbatively controlled in $J(\boldsymbol{k})/T$.

- Aim of flow: Extrapolate from controlled high-T regime to low temperatures $T \ll J(\boldsymbol{k})$ by resumming classes of diagrams.

  $\Rightarrow$ $T < J(\boldsymbol{k})$ regime requires nonperturbative truncation!

$T \to 0$ description of quantum antiferromagnets

- Frustrated interactions or reduced dimensions:
  Spin-length constraint $\boldsymbol{S}_i^2 = S(S+1)$ expected to be important.

- Example: 2-dimensional quantum antiferromagnet;
  successfully described at low temperatures by nonlinear σ model
  [Chakravarty PRB 1989, Chubukov PRB 1994, ...],

$$\mathcal{Z} \propto \int \mathcal{D}\hat{\boldsymbol{n}}(\boldsymbol{x},\tau)\delta\left(|\hat{\boldsymbol{n}}|-1\right) e^{-\frac{\rho}{2}\int_0^\beta \mathrm{d}\tau \int \mathrm{d}^2x \left(|\nabla\hat{\boldsymbol{n}}|^2 + |\partial_\tau \hat{\boldsymbol{n}}|^2/c^2\right)} ,$$

  interacting *only* through spin-length constraint.

⇒ Implies importance of susceptibility sum rule

$$\langle \boldsymbol{S}_i(\tau)\cdot\boldsymbol{S}_i(\tau)\rangle = 3G_{ii}(\tau,\tau) = 3\int_{\boldsymbol{k},\omega} G(\boldsymbol{k},\omega) = S(S+1)\ .$$

- However, the spin-length constraint likewise implies

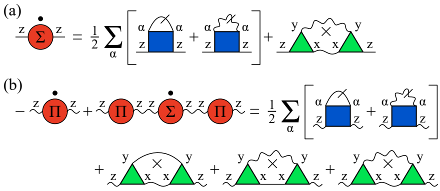
$$\begin{aligned}\left\langle \mathcal{T} S_i^x(\tau) S_j^x(\tau') \boldsymbol{S}_n(\tau'')\cdot\boldsymbol{S}_n(\tau'')\right\rangle &= G_{ij}(\tau,\tau')S(S+1) \\ &= 3G_{ij}(\tau,\tau')G_{nn}(\tau'',\tau'')\ ,\ldots\end{aligned}$$

2-spin sum rules of the hybrid functional

- 2-spin flow equations:

$$\partial_\Lambda \Sigma_\Lambda(\boldsymbol{k}) = -T \int_{\boldsymbol{q}} \left[\partial_\Lambda J_\Lambda(\boldsymbol{q})\right] G_\Lambda^2(\boldsymbol{q}) \times \left[\Gamma_\Lambda^{(4)}(\boldsymbol{k},\boldsymbol{q}) + \gamma_\Lambda(\boldsymbol{k},\boldsymbol{q})\right] ,$$

$$-\partial_\Lambda \Pi_\Lambda(K) + \Pi_\Lambda^2(K)\partial_\Lambda \Sigma_\Lambda(\boldsymbol{k}) = -T \int_{\boldsymbol{q}} \left[\partial_\Lambda J_\Lambda(\boldsymbol{q})\right] G_\Lambda^2(\boldsymbol{q}) \tilde{\gamma}_\Lambda(K,\boldsymbol{q}) .$$



[γ_Λ, $\tilde{\gamma}_\Lambda$: dynamical diagrams encoding quantum fluctuations; wavy lines]

⇒ Associated sum rules:

$$1 = T \int_{\boldsymbol{q}} G_\Lambda^2(\boldsymbol{q}) \left[\Gamma_\Lambda^{(4)}(\boldsymbol{k},\boldsymbol{q}) + \gamma_\Lambda(\boldsymbol{k},\boldsymbol{q})\right] , \qquad \Pi_\Lambda^2(K) = T \int_{\boldsymbol{q}} G_\Lambda^2(\boldsymbol{q}) \tilde{\gamma}_\Lambda(K,\boldsymbol{q}) .$$

[equivalent to $\langle \mathcal{T} S_i^x(\tau) S_j^x(\tau') \boldsymbol{S}_n(\tau'') \cdot \boldsymbol{S}_n(\tau'') \rangle = G_{ij}(\tau,\tau') S(S+1)$]

Nonperturbative truncation

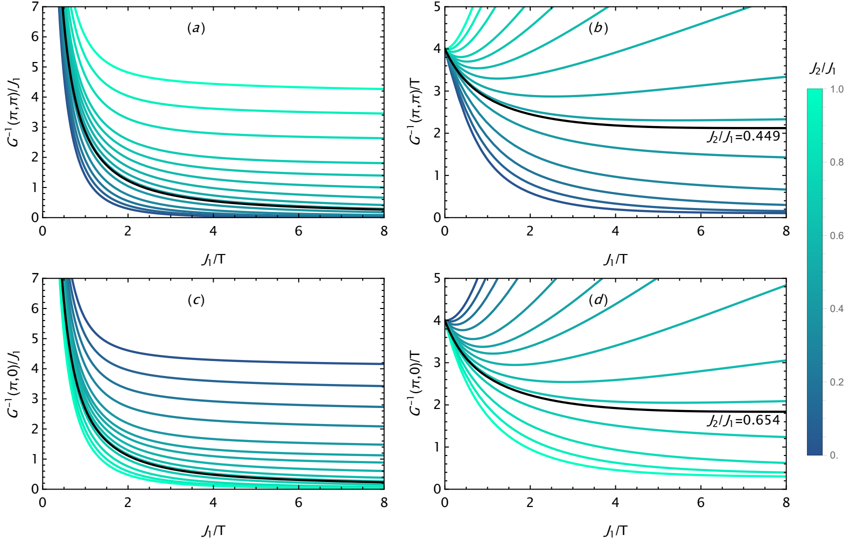
- Strategy: Fix 3- and 4-spin vertices via sum rules and spin algebra.
- Ansatz for statics: $\Gamma_\Lambda^{(4)}(\boldsymbol{k},\boldsymbol{q}) = U_\Lambda + [V_\Lambda(\boldsymbol{k}) - 1]\,\gamma_\Lambda(\boldsymbol{k},\boldsymbol{q})$.
  - U_Λ fixed by demanding $\partial_\Lambda \int_K G_\Lambda(K) = 0$.
  - $V_\Lambda(\boldsymbol{k})$: quantum correction required to also satisfy static 2-spin sum rule $1 = T\int_{\boldsymbol{q}} G_\Lambda^2(\boldsymbol{q})\left[\Gamma_\Lambda^{(4)}(\boldsymbol{k},\boldsymbol{q}) + \gamma_\Lambda(\boldsymbol{k},\boldsymbol{q})\right]$.
- Dynamic vertices from equations of motion neglecting loops.
  - Includes spin algebra and spin conservation nonperturbatively.

$\Rightarrow$ Nonperturbative closure on 2-spin level.

- Additionally: high-frequency approximation $\Pi_\Lambda(\boldsymbol{k},\omega) \approx A_\Lambda(\boldsymbol{k})/\omega^2$.
- At large frustration: unphysical $A_\Lambda(\boldsymbol{0}^+) < 0$ at low temperatures.

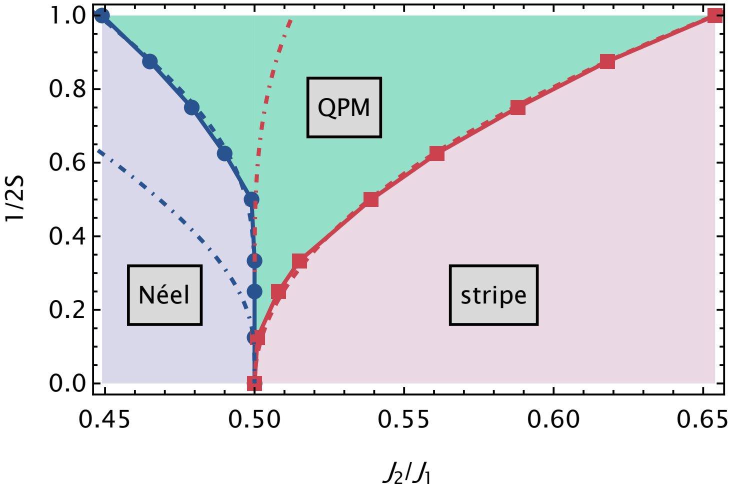
  $\Rightarrow$ Flow breaks down eventually.

Flow of the spin gap of the J_1-J_2 model for $S = 1/2$



- $T = 0$ phase transition: $G^{-1}(\boldsymbol{Q})/T$ flat for $1/T \to \infty$.

Phase diagram of the J_1-J_2 model for arbitrary spin



- Quantum paramagnet disappears for $S \gtrsim 5$.
- Phase boundaries qualitatively similar to spin wave theory, but large quantitative difference for small S.

Conclusions & outlook

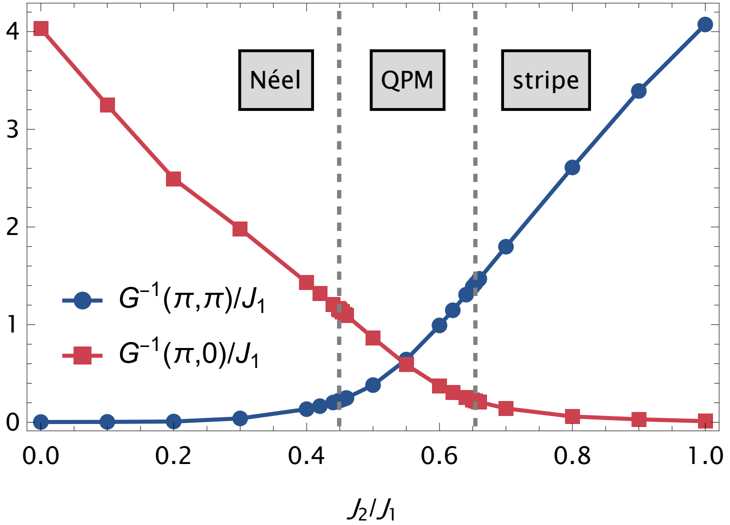
- Technical advances:
  1. Spin-length constraint $\boldsymbol{S}_i^2 = S(+1) \Rightarrow$ infinite tower of sum rules, one for each flow equation.
  2. Sum rules, spin algebra & ergodicity are crucial for nonperturbative truncations applicable to frustrated magnets in reduced dimensions.
  3. Good results can be obtained with low numerical costs.
  4. Arbitrary S without any additional complications.

- Main physical result: Phase diagram of J_1-J_2 antiferromagnet on the square lattice at arbitrary S.

- Future research:
  1. More complicated frustrated models, magnetic fields . . .
  2. 4-spin correlations to characterize quantum paramagnetic phases.
  3. Keldysh spin FRG.

A. Rückriegel, D. Tarasevych, and P. Kopietz,
Phys. Rev. B **109**, 184410 (2024)

Residual spin gaps of the J_1-J_2 model for $S = 1/2$



- Final temperature in strongly frustrated region too large to detect possible first order transition.

Spin-length constraint in the spin FRG

- To elegantly derive spin-length sum rules for vertices from the hierarchy of spin FRG flow equations, rewrite

$$
\begin{aligned}
\mathcal{H}_\Lambda &= \frac{1}{2}\sum_{ij} J_{ij}^\Lambda \boldsymbol{S}_i \cdot \boldsymbol{S}_j \\
&= \frac{1}{2}\sum_{ij} \left(J_{ij}^\Lambda + \delta_{ij} C_\Lambda - \delta_{ij} C_\Lambda \right) \boldsymbol{S}_i \cdot \boldsymbol{S}_j \\
&= \frac{1}{2}\sum_{ij} \left(J_{ij}^\Lambda + \delta_{ij} C_\Lambda \right) \boldsymbol{S}_i \cdot \boldsymbol{S}_j - \frac{N}{2} C_\Lambda S(S+1) \,.
\end{aligned}
$$

Crucial observations

- No modification to the system at all, only added a zero.

$\Rightarrow$ All correlation functions remain unchanged and independent of C_Λ.

- However, flow equations modified non-trivially!

Spin-length constraint in the spin FRG

- Modification of the flow of the generating functional of connected spin correlation functions:

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

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

$$+ \frac{\beta N}{2}\partial_\Lambda C_\Lambda S(S+1) \, .$$

$\Rightarrow$ Sum rule for the generating functional:

$$S(S+1) = \frac{1}{\beta N}\int_0^\beta \mathrm{d}\tau \sum_{i,\alpha} \left[\frac{\delta^2 \mathcal{G}_\Lambda[h]}{\delta h_i^\alpha(\tau)\delta h_i^\alpha(\tau)} + \frac{\delta \mathcal{G}_\Lambda[h]}{\delta h_i^\alpha(\tau)} \frac{\delta \mathcal{G}_\Lambda[h]}{\delta h_i^\alpha(\tau)}\right] \, .$$

Implies infinite tower of sum rules, one for each flow equation.

Spin-length constraint in the spin FRG

- Sum rules and flow equations have the same structure.
- Invariance of physical functions under shift $J_\Lambda(\boldsymbol{k}) \to J_\Lambda(\boldsymbol{k}) + C_\Lambda$ implies simple translation rules from flow equations to sum rules.
- Hybrid functional: All vertex functions are defined in terms of physical spin correlation functions.
  - Only exception: static spin self-energy $\Sigma_\Lambda(\boldsymbol{k}) = G_\Lambda^{-1}(\boldsymbol{k}) - J_\Lambda(\boldsymbol{k})$.

$\Rightarrow$ Hybrid functional translation rules:

flow equation $\to$ sum rule

(i) $\partial_\Lambda J_\Lambda(\boldsymbol{k}) \to 1$,

(ii) $\partial_\Lambda \Sigma_\Lambda(\boldsymbol{k}) \to -1$,

(iii) $\partial_\Lambda f_\Lambda \to S(S+1)/2$,

(iv) all other ∂_Λ-terms $\to 0$.