Spin functional renormalization group for dimerized quantum spin systems

Andreas Rückriegel

Institut für Theoretische Physik, Universität Frankfurt

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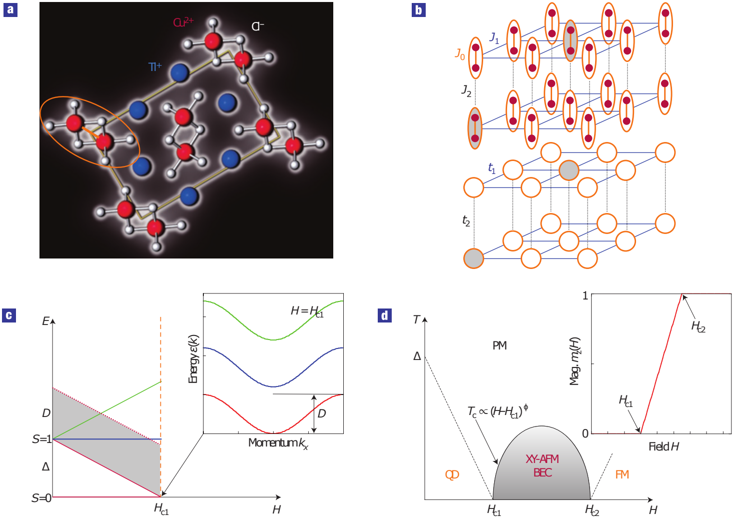
Dimerized quantum spin systems



[Giamarchi, Rüegg, Tchernyshyov, Nature Phys. **4**, 198 (2008)]

Dimerized quantum spin systems

- Hamiltonian:

$$\mathcal{H} = \sum_{i=1}^{N} h_i + \mathcal{V} \,, \qquad h_i = A\boldsymbol{s}_{i,1} \cdot \boldsymbol{s}_{i,2} - H \left(s^z_{i,1} + s^z_{i,2} \right) \,.$$

- Inter-dimer exchange:

$$\mathcal{V} = \frac{1}{2} \sum_{ij} \Big(J^{\perp}_{T,ij} \boldsymbol{T}^{\perp}_i \cdot \boldsymbol{T}^{\perp}_j + J^{\parallel}_{T,ij} T^z_i T^z_j + J^{\perp}_{S,ij} \boldsymbol{S}^{\perp}_i \cdot \boldsymbol{S}^{\perp}_j + J^{\parallel}_{S,ij} S^z_i S^z_j \Big) \,.$$

$$\boldsymbol{S}_i = \boldsymbol{s}_{i,1} + \boldsymbol{s}_{i,2}$$
$$\boldsymbol{T}_i = \boldsymbol{s}_{i,1} - \boldsymbol{s}_{i,2}$$
$$|J^{\alpha}_{a,ij}| < A$$

Spin FRG approach: Continuously deform exchange couplings

$$J^{\alpha}_{a,ij} \to J^{\alpha}_{\Lambda,a,ij} \,, \quad \Lambda \in [0,1] \,,$$

such that

1. $J^{\alpha}_{\Lambda=0,a,ij} = 0$ (decoupled dimers),
2. $J^{\alpha}_{\Lambda=1,a,ij} = J^{\alpha}_{a,ij}$ (full interacting system).

Spin functional renormalization group

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$\Rightarrow$ 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.
- Non-trivial initial conditions because of $SU(2)$ spin algebra.

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

Spin dimer

- Two coupled $s = 1/2$ spins:

$$h = A\boldsymbol{s}_1 \cdot \boldsymbol{s}_2 - H\left(s_1^z + s_2^z\right) \ .$$

  - $A > 0$ (antiferromagnetic)

- Eigenenergies (up to a constant):

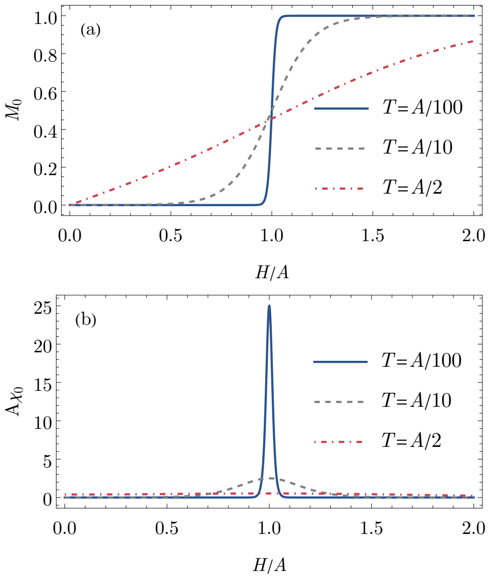
$$E^s = 0 \ ,$$

$$E^+ = A - H \ ,$$

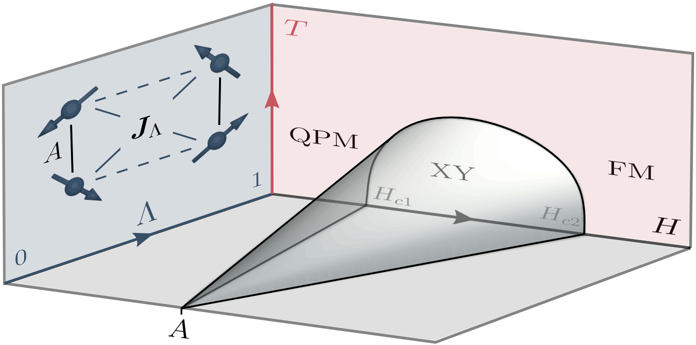
$$E^0 = A \ ,$$

$$E^- = A + H \ .$$

- Quantum critical point at $H = A$.



Flow of the phase diagram



- Dimer QCP grows into XY antiferromagnetic phase in $D = 3$.
- Two BEC quantum phase transitions at H_{c1} and H_{c2}.

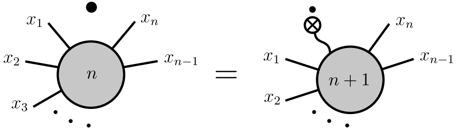
Truncation

- Tadpole diagrams:

  self-consistent mean-field theory,

  $$H \to H - J^{\|}_{\Lambda,S,\boldsymbol{k}=0} M_\Lambda \ ;$$

  "flowing chemical potential".

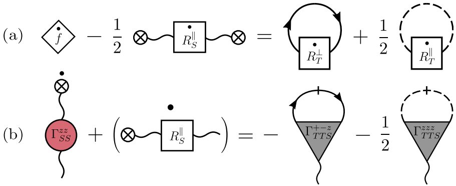


- Loop-integrations:

  $\propto$ (inter-dimer exchange)^2.

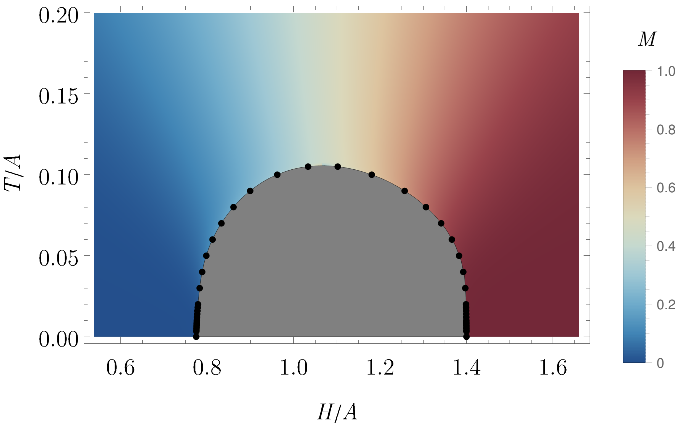
- 1-loop approximation:

  random-phase approximation for inter-dimer exchange.



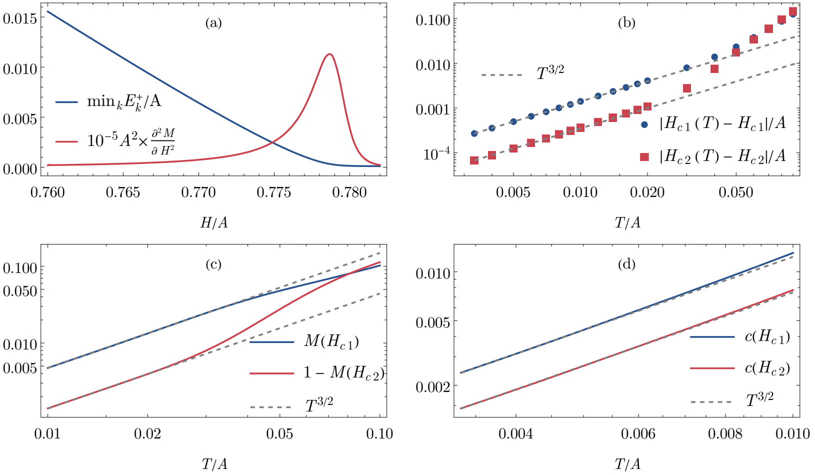
$\Rightarrow$ Ordinary differential equations for magnetization M_Λ, free energy f_Λ, ...

1-loop phase diagram



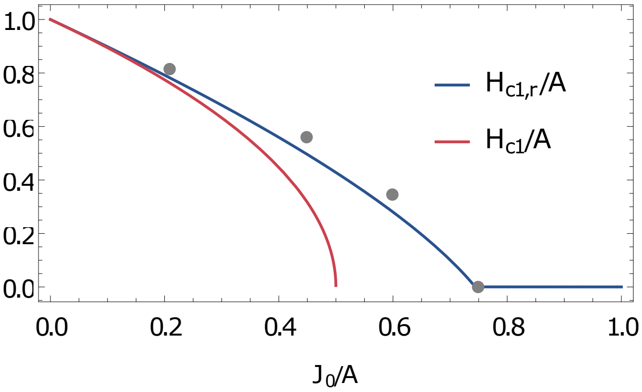
- Shaded area: XY-order, flow equation becomes unphysical.
  - Reason: No finite $\langle T_i^{\pm} \rangle$ taken into account.

Critical exponents



- Correct power laws for BEC quantum critical points in $D = 3$.

Quantum fluctuations at $T = 0$



- Lower quantum critical field renormalized: $H_{c1} \to H_{c1,r}$.
- Agrees well with QMC data (gray circles).

  [Nohadani *et al.*, Phys. Rev. B **69**, 220402(R) (2004)]

Conclusions & outlook

- Spin functional renormalization group:

  1. Useful new tool for analytical & nonperturbative calculations in quantum spin systems.
  2. Simple truncations can already yield quantitatively accurate results with modest numerical effort.

- Outlook:

  1. XY-ordered phase
  2. Quantum critical fluctuations & damping
  3. Frustration

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