funRG at all scales: the charge-density wave problem

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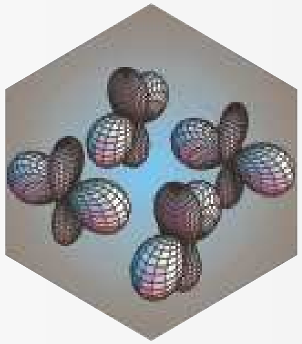
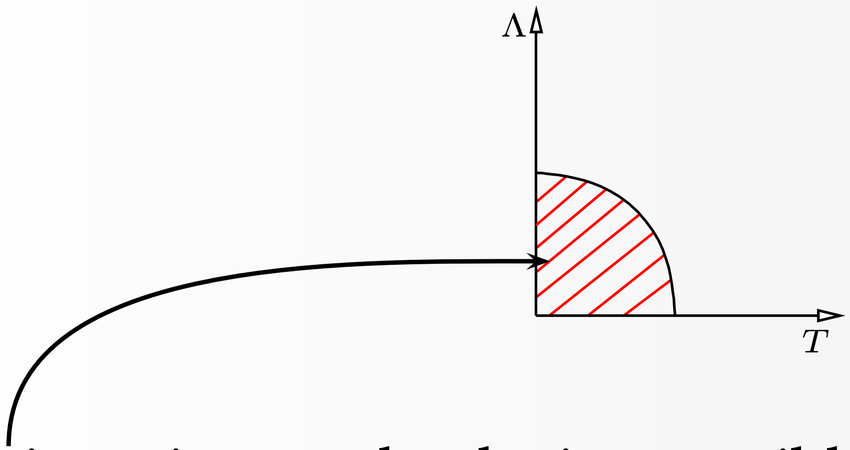


[1] now Würzburg [2] now Paris

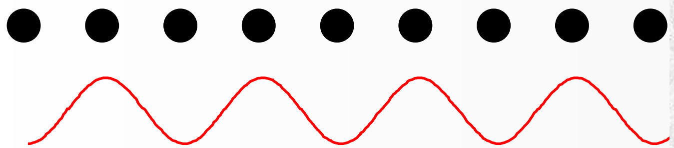
Why?

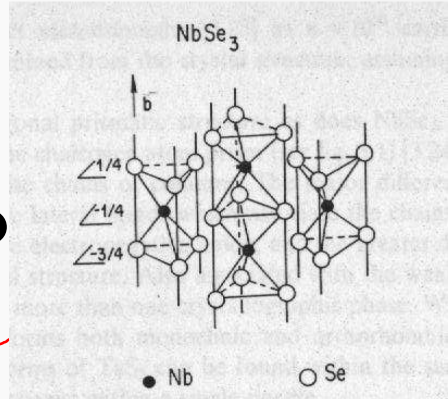


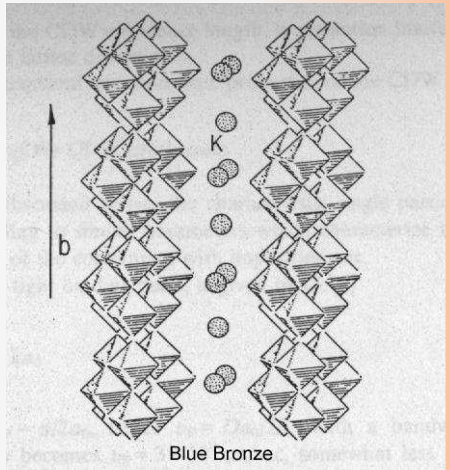
- This region used to be inaccessible to funRG techniques.
- funRG techniques used to be unable to reproduce mean-field results for mean-field-exact models.

Here, we employ an improved funRG (Katanin scheme) and an initial symmetry-breaking field in a charge-density-wave system.

- 1d atomic lattice: oscillating electron density at low temperatures due to Peierls distortion.







Images from Grüner and Zettl, 1984

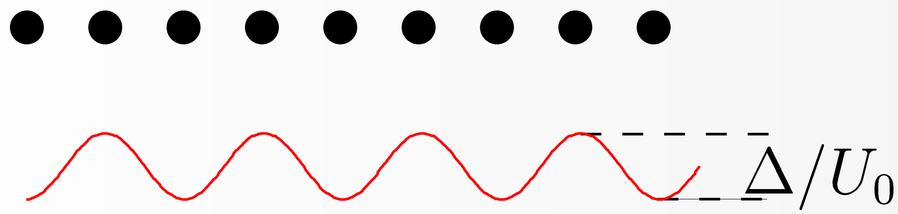
- CDWs are experimentally observed in various compounds, e.g. $NbSe_3$, TaS_3, blue bronze ($K_{0.3}MoO_3$), $(TaSe_4)_2I$.

  Transition temperatures: from 24K ($Li_{0.9}Mo_6O_{17}$) up to 793K ($NbTe_4$).

- One-dimensionality arises from the crystal structure.

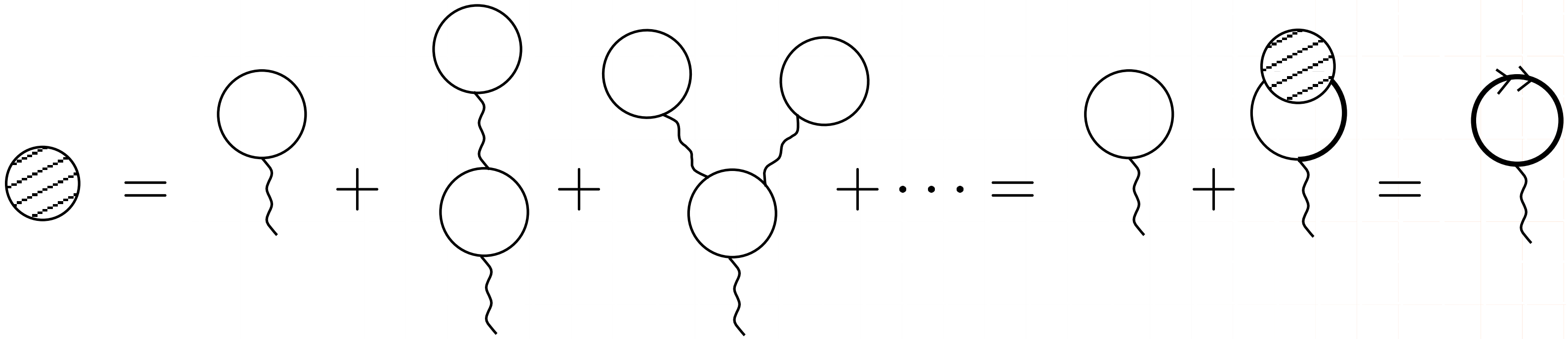
Formal Matters

- We start from a model where particles can *hop* and *repel* each other: $H' = -t\sum_i (c_i^\dagger c_{i+1} + h.c.) + U_0 \sum_i n_i n_{i+1}$.

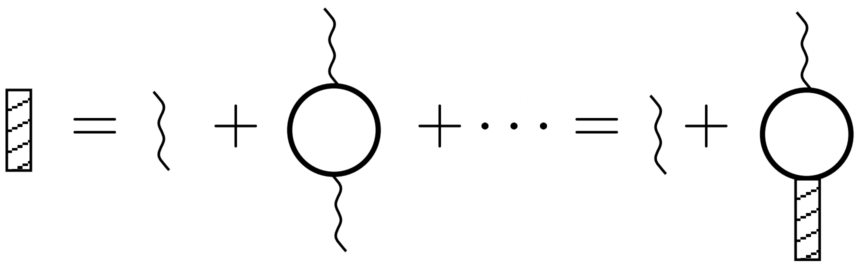


- Leadingly divergent at half-filling: π-transferring processes that generate the CDW.
  $H = \sum_k \varepsilon_k n_k - \frac{U_0}{N} \sum_{k,k'} c_k^\dagger c_{k+\pi} c_{k'}^\dagger c_{k'+\pi}$
- Thermodynamic limit, half-filling.
- Δ/U_0: amplitude of the density wave. Referred to as gap, off-diagonal self-energy, pairing field or order parameter.
  U: vertex, effective interaction, effective coupling or four-point-function.
  Δ and U take real values and depend only on Λ and T.

- Exact in the thermodynamic limit: derivation of the gap equation by resummation.

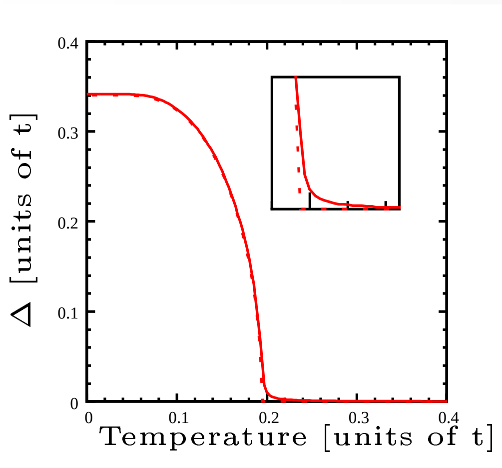


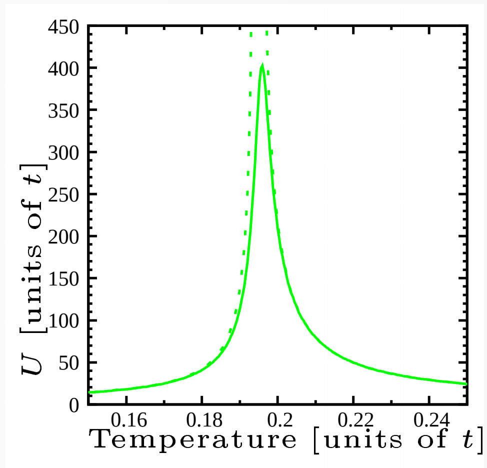
- Likewise, we can resum for the effective interaction.



Exact Results

- Exact in the thermodynamic limit: derivation of the gap equation by resummation.



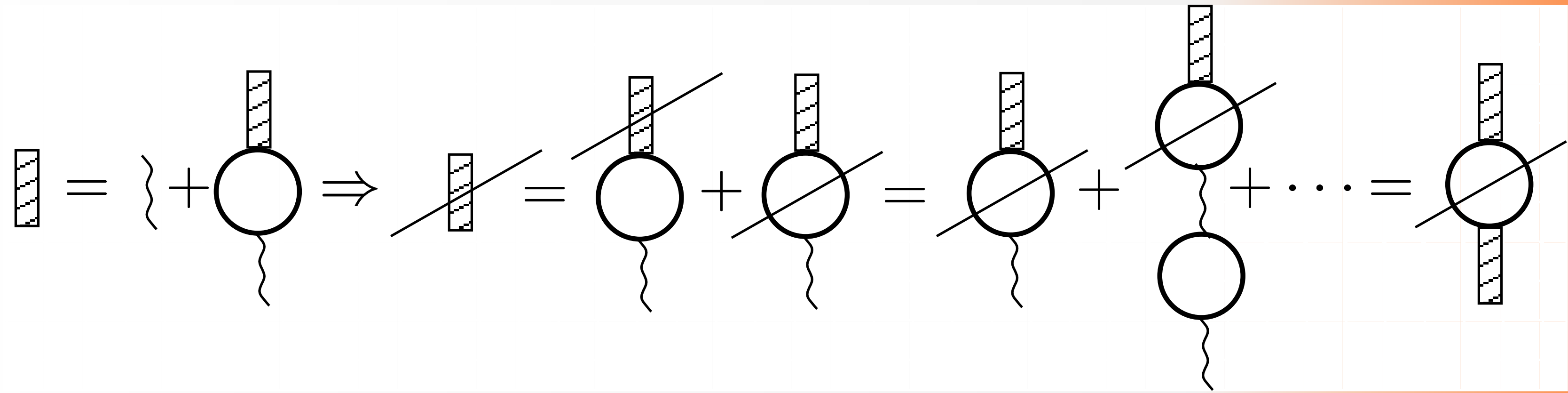


$$U = \frac{U_0}{1 - U_0 \mathrm{Bubble}}$$

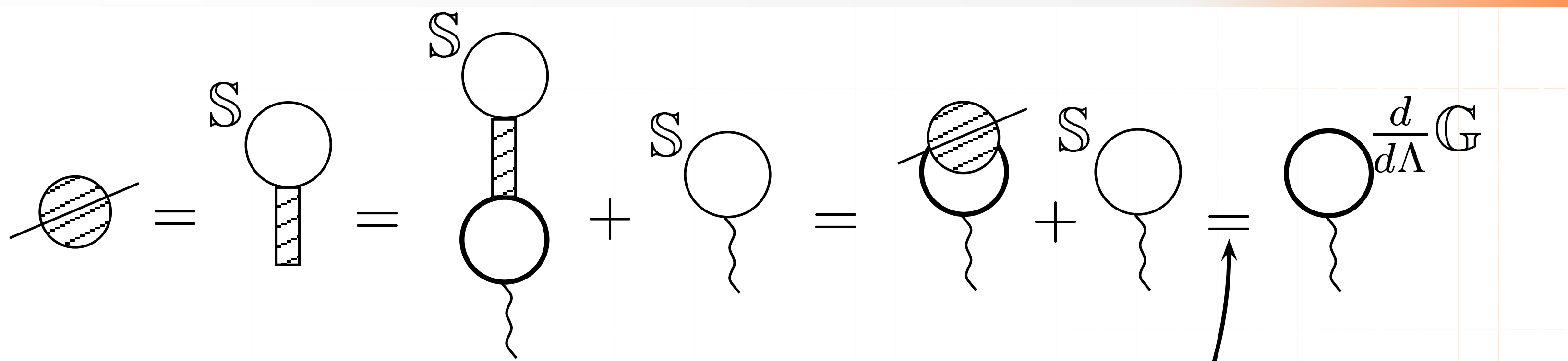
- Likewise, we can resum for the effective interaction.
- We introduce a small initial gap. The phase transition is "smeared out" and the singularity of the effective interaction is regularized.

funRG equations

- Vertex flow equation from Bethe-Salpeter equation:



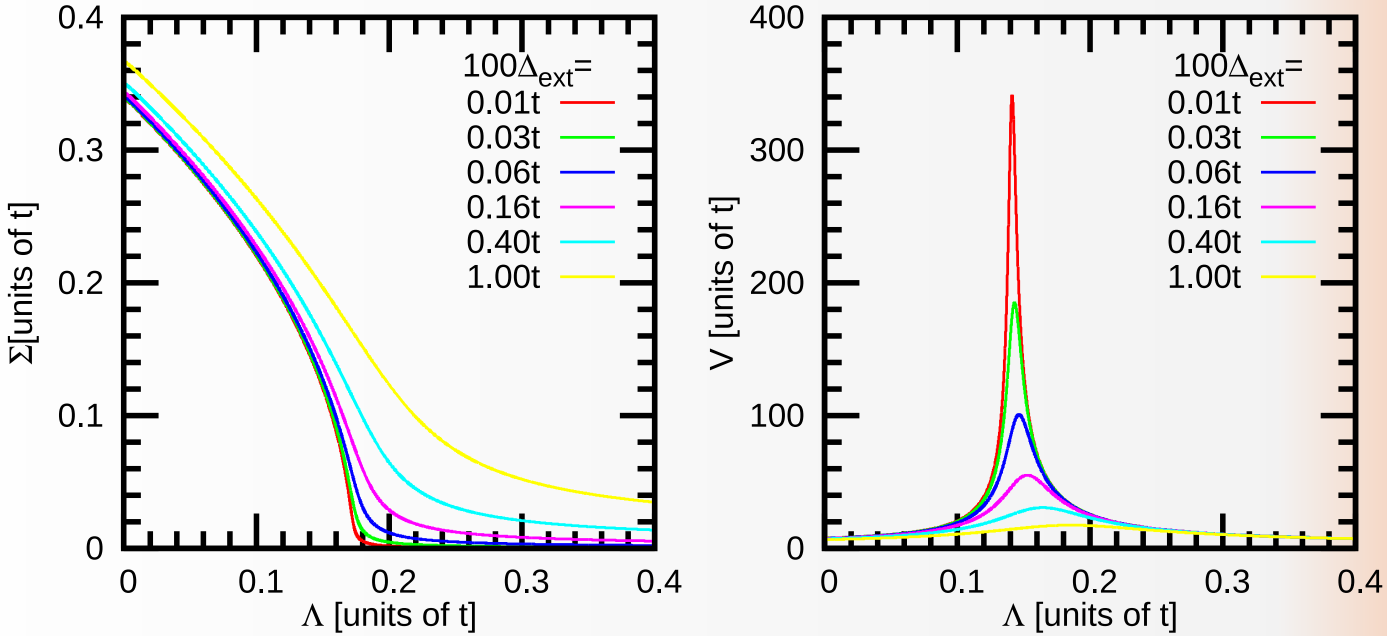
- Gap flow equation from gap equation, $\mathbb{S} := -\mathbb{G}\frac{d}{d\Lambda}\mathbb{G}_0^{-1}\mathbb{G}$:



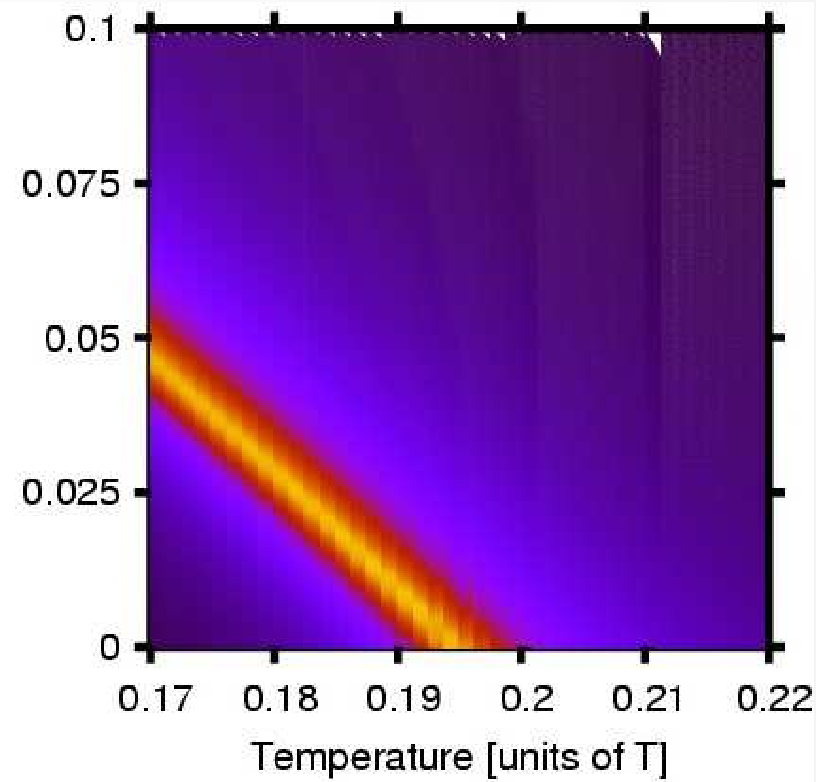
$$-\mathbb{G}\frac{d}{d\Lambda}\mathbb{G}_0^{-1}\mathbb{G} + \mathbb{G}\frac{d}{d\Lambda}\Sigma\mathbb{G} = -\mathbb{G}\frac{d}{d\Lambda}\mathbb{G}^{-1}\mathbb{G} = \frac{d}{d\Lambda}\mathbb{G}$$

Exact Results (funRG)

- The sub-T_c flows of the effective interaction and the gap resemble the temperature dependences.



- Increasing the initial gap suppresses the effective interaction flow maximum and furthers the smearing of the transition.
- The final value of the self-energy changes by only 10% while the initial gap varies over two orders of magnitude!



Temperature dependence of the effective interaction flow around the critical temperature: The flow maximum is pushed linearly towards zero scale by increasing temperature.

Summary and Outlook

- Katanin-funRG + small external gap reproduce exact results for self-energy and effective interaction in the CDW-model at all temperatures. The scheme is implemented numerically at fairly high precision.
- We will next look at models with two interaction processes. The medium-long term goal is to describe competing instabilities. This appears feasible away from critical points since we can strongly suppress the effective interaction flow without contracting a large error in the $\Lambda = 0$ results.

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