Max-Planck-Institut für
Struktur und Dynamik der Materie

Parquet approach - the most fundamental diagrammatic method?

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Parquet approach - the most fundamental diagrammatic method?

→ **It is *very* fundamental**

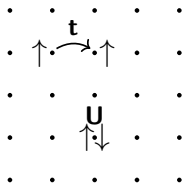
C.E. et al. - in preparation

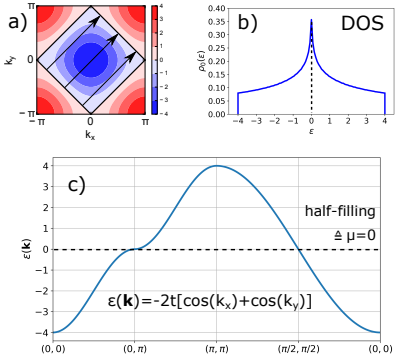
→ **It is now doable for relevant system sizes**

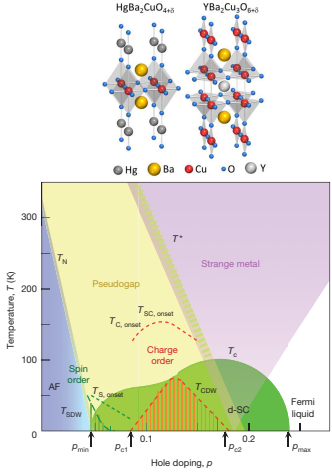
C.E. et al. Rev. B 101, 155104, (2020)
T. Schäfer et al. arXiv:2006.10769 - to appear in PRX, (2021)

The 2D Hubbard model

$$H = -t \sum_{\langle i,j \rangle} \sum_{\sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} + U \sum_{i,\sigma} n_{i,\sigma} n_{i,-\sigma}$$





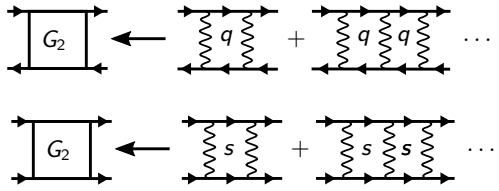


B. Keimer et al. - Nature 518, Feb. 2015

How to tackle problem? $\rightarrow$ **Diagrammatic point of view**

Goal: Calculate $G_{2\text{particle}}$

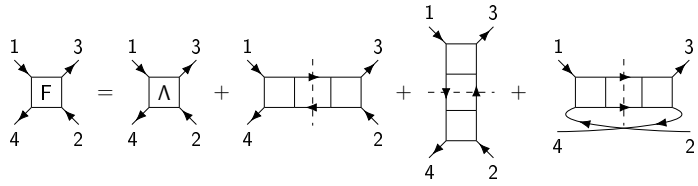
Challenge: Competing orders



How to tackle problem of correlated electrons?

→ parquet

$$G_{\text{2particle}} = GG + GG\,F\,GG$$



$$F = \Lambda + \Phi_{ph} + \Phi_{\overline{ph}} + \Phi_{pp}$$

→Iterative method to calculate Σ and F consistently

Is parquet the *most fundamental* diagrammatic method?

Answer: It is very fundamental!

1. **Reason:** Very fundamental derivation possible!

$$\text{Action} + \text{Legendre transform} = \ldots \text{lots of algebra} \cdots = \text{parquet equation}$$

C.E., P. Kauch, A. Kauch, K. Held - in preparation

2. **Reason:** Many diagrammatic methods try to approximate parquet
   - fRG - 2^{nd}truncation
     F. Kugler and J. von Delft 2018 New J. Phys. 20 123029
     C. Hille et al. Phys. Rev. Research 2, 033372 Published 8 September 2020
   - GWγ
     F. Krien, A.Kauch, K. Held 2020 arXiv:2009.12868
   - Diagrammatic extensions of DMFT
     G. Rohringer et al. Rev. Mod. Phys. 90, 025003 2018

Parquet's *big* problem:

Memory Consumption!

Bad scaling: $F^{k_1,k_2,q} \rightarrow \mathcal{O}(N_k^3 \times N_\omega^3)$

'Small' example:

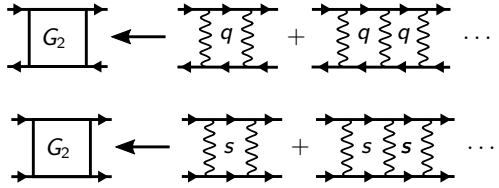
$$N_x \times N_y = (10 \times 10); \quad N_\omega = 100 \Rightarrow F \sim 16\text{TB}$$

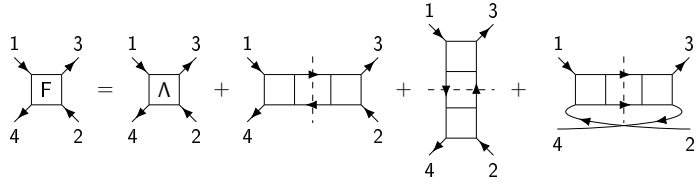
$\rightarrow$previously reachable system sizes: 8×8 grid ($>$ 5 TB of memory)

G. Li et al. - Comput. Phys. Commun. 241 (2019)

S. Yang et al. - Phys. Rev. E (2009)

Try to extract the relevant physics - Extra approximation

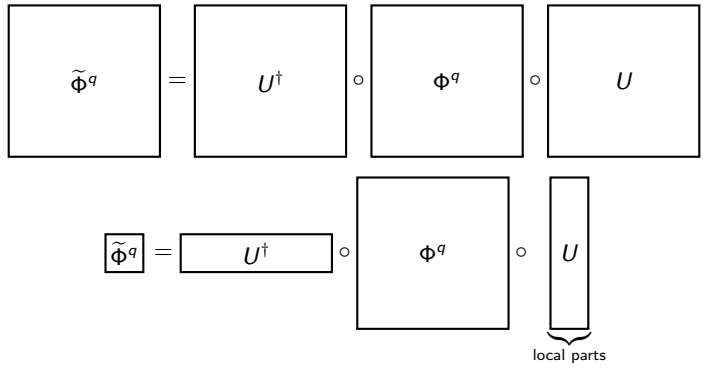




$$F = \Lambda + \Phi_{ph} + \Phi_{\overline{ph}} + \Phi_{pp}$$

Truncated Unity approximation

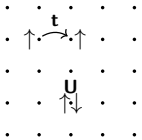
$$\Phi^{k_1,k_2,q} = \underline{\underline{\Phi}}^q = \underline{\underline{U}}^\dagger \underline{\underline{\widetilde{\Phi}}}^q \underline{\underline{U}} =: \widetilde{\Phi}^{\ell_1,\ell_2,q}$$

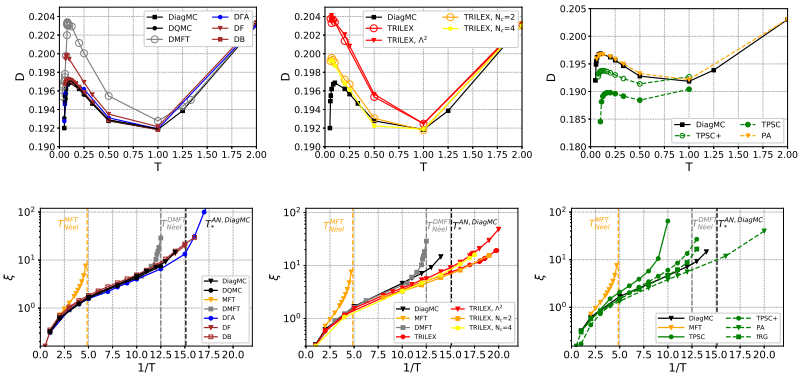


$$\mathcal{O}((N_k \times N_\omega)^3) \to \mathcal{O}((N_\omega)^3 \times N_k \times N_{FF}^2)$$

C.E. et al. Phys. Rev. B 98, (2018)
C.E. et al. Phys. Rev. B 101, (2020)

Parquet is now a competitive many-body method!

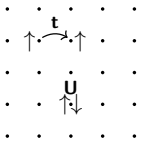


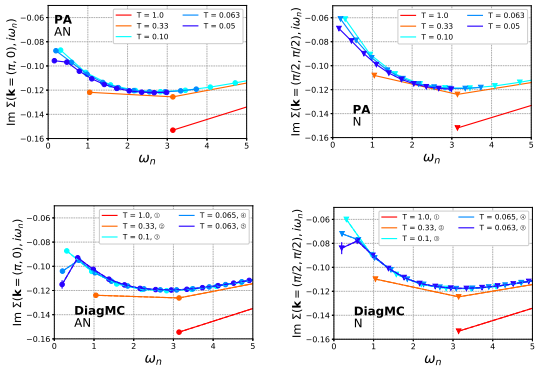


Double occupancies (top) and AF correlation lengths (bottom)

T. Schäfer et al. arXiv:2006.10769 $\longrightarrow$ to appear in PRX

We are able to reproduce the pseudogap

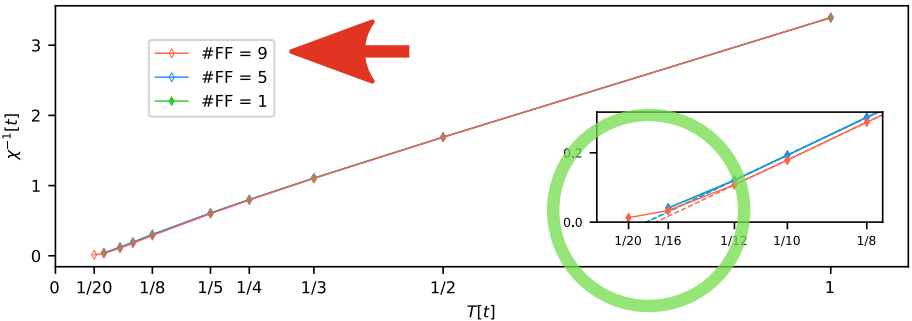




→Able to study origin of peusdogap

C. Hille et al. Phys. Rev. Research 2, (2020)

Inverse AF susceptibility



First indication of fulfillment of Mermin-Wagner with parquet

C.E. et al. Phys. Rev. B 101, (2020)

Parquet approach - the most fundamental diagrammatic method?

→ **It is *very* fundamental**
Can be derived from fundamental priciples
Other methods try to approximate it

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Many thanks to ...

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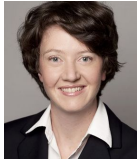

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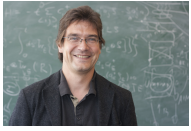

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