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Single Boson Exchange fRG for Extended Interactions: A Handy Computational Scheme

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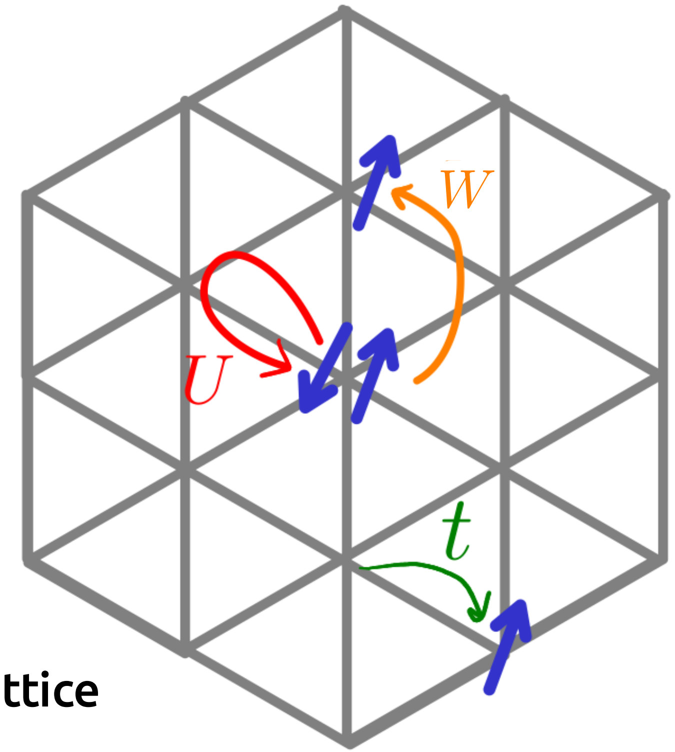
Hubbard Model

J. Hubbard (1963)

"Fermions hopping on a lattice"

$$\mathcal{H} = \sum_{i \neq j, \sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \frac{1}{2} \sum_{i,j,\sigma,\sigma'} V_{0,ij} n_{i\sigma} n_{j\sigma'} - \mu \sum_{i,\sigma} n_{i\sigma}$$



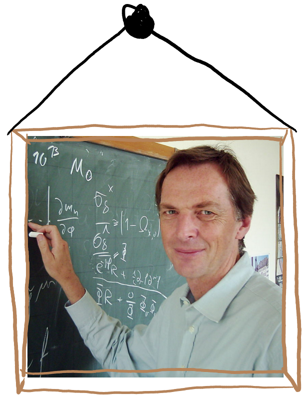
Why extended?

- More realistic; Coloumb interactions not completely screened.
- Onsite ~> AFM fluctuations, extended ~> CDW fluctuations.
  AFM - CDW transition at low T. Bari et al (1971)
- Moire heterobilayers of TMDs ~> Single band on triangular lattice with extended interactions. F. Wu et al (2018)
- Electron - Phonon couplings are non-local in time ~> competition between conventional and unconventional superconductivity.

fRG promotional

"Interpolate between a solvable and a more difficult theory"

e.g. by deforming $\mathcal{G}_0 \rightsquigarrow \mathcal{G}_{0,t}$



Tower of flow equations for the 1PI vertices:

$$\partial_t \Gamma_t^{(2n)} = \mathcal{F}[\Gamma_t^{(2n+2)}, \cdots, \Gamma_t^{(2)}]$$

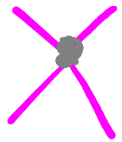
Truncation:

$$\partial_\lambda \Gamma_\lambda^{(2n)} = 0 \quad \text{for} \quad n \geq 3 \rightsquigarrow \textbf{state: } \vec{\psi} = \begin{pmatrix} \Sigma \\ V \end{pmatrix} \rightsquigarrow \text{Solve numerically}$$

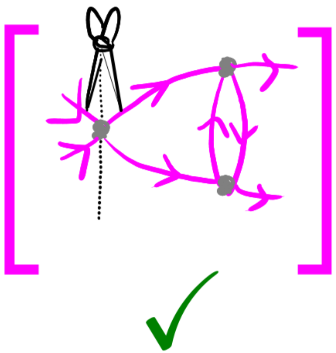
Sales pitch:

- treatment of channels $\rightsquigarrow$ no bias
- frustration or finite doping at low T $\rightsquigarrow$ no problem
- d > 1 $\rightsquigarrow$ no fundamental limitations
- 2P consistency $\rightsquigarrow$ extensions (multiloop) F. Kugler et al (2018)
- Strong coupling $\rightsquigarrow$ extensions (DMF2RG) C. Taranto et al (2014)

Single Boson Exchange Decomposition

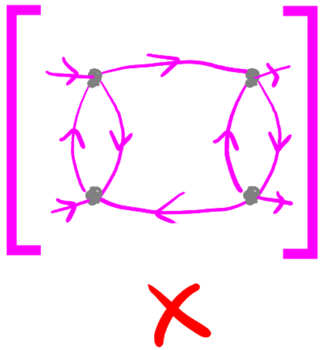
Bare interaction: $V_0 = U\delta(\sum k_i = 0) \mathrel{\hat{=}}$ 

Bare interaction (U)-reducibility ($X \in \{pp, ph, xph\}$):



$\in \sum_X \nabla^X$

"Single boson exchange contributions"



$\in \sum_X M^X$

The 2PR multiboson contributions ;the "rest function"

SBE decomposition:

$$V = \sum_X \nabla^X + \sum_X M^X - 3V_0 + V_{2PI}$$

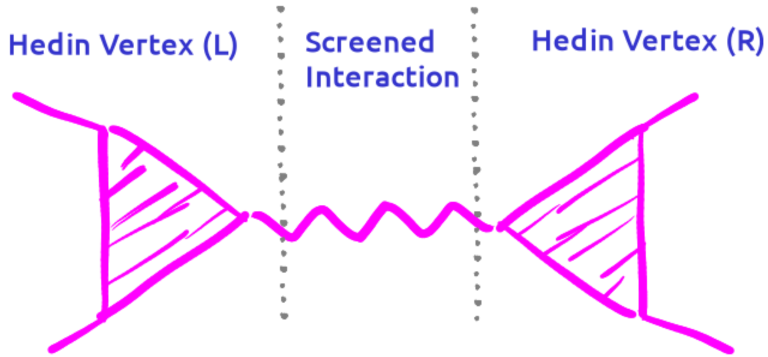
set to V_0

Single Boson and Multi Boson Exchanges

Factorise

$$\nabla^X(q,k,k') = \lambda^X(k,q)\cdot w^X(q)\cdot \bar{\lambda}^X(k',q)$$

$\hat{=}$



"single boson exchange"

Can show:

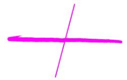
$$\lambda^X = \bar{\lambda}^X$$

Everything else: M^X "multi boson exchanges"

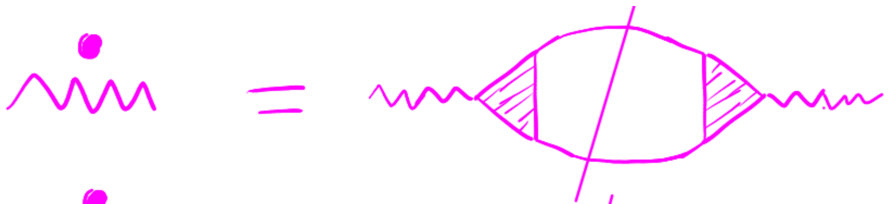
$$V = \sum_X \nabla^X + \sum_X M^X - 3V_0 + V_{2PI}$$

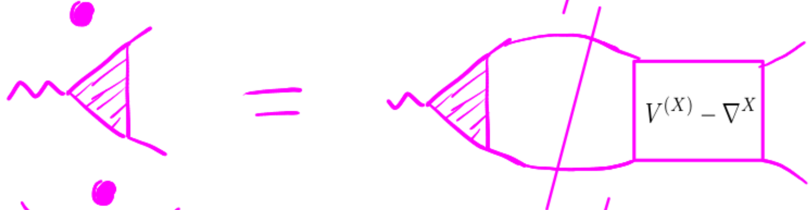
SBE 1-loop flow equations

P. Bonetti et al (2022)

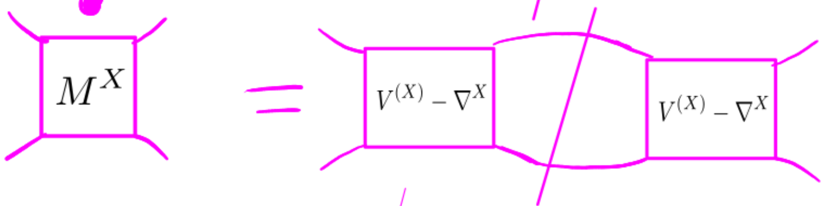
Flow equations (with $\left.\frac{\partial}{\partial t}\mathcal{G}\right|_{\Sigma=\text{const}} \mathrel{\hat{=}}$ )

Plug in SBE decomposed vertex, use properties of w^X, λ^X, M^X

$\partial_t w^X(q) \;\hat{=}$  with $w^X_{t=0} = V_0^{(X)}$

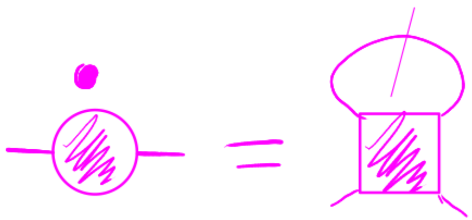
$\partial_t \lambda^X_k(q) \;\hat{=}$ 

with $\lambda^X_{t=0} = 1$

$\partial_t M^X_{k,k'}(q) \;\hat{=}$ 

with $M^X_{t=0} = 0$

standard SE flow equation

$\partial_t \Sigma_k \;\hat{=}$  with $\Sigma_{t=0} = 0$

Frequency Dependence and Self-Energy

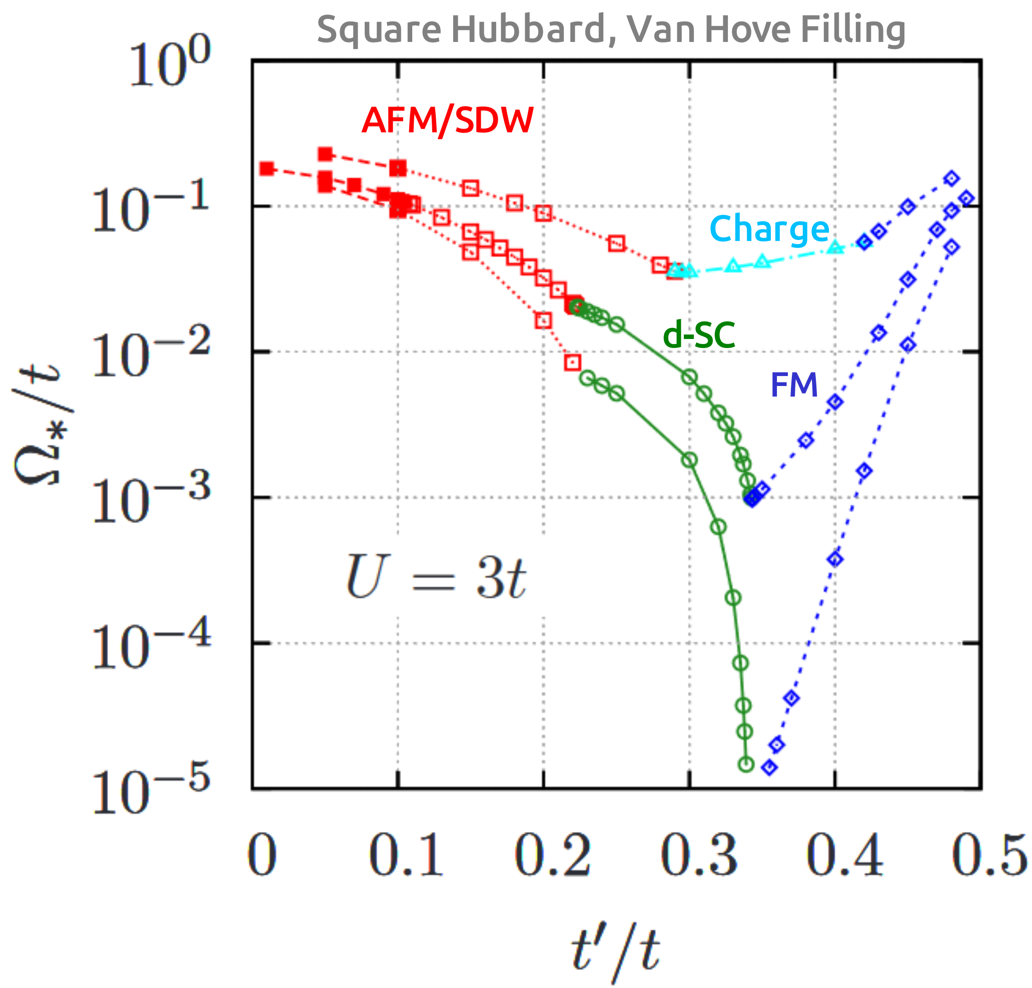
Naive power counting argument:

frequency dependent parts of vertex are irrelevant

From top to bottom:

- $V(\omega)$ $\cancel{\Sigma(\omega)}$
- $V(\cancel{\omega})$ $\cancel{\Sigma(\omega)}$
- $V(\omega)$ $\Sigma(\omega)$

$\rightsquigarrow$ A quantitative and a qualitative difference!



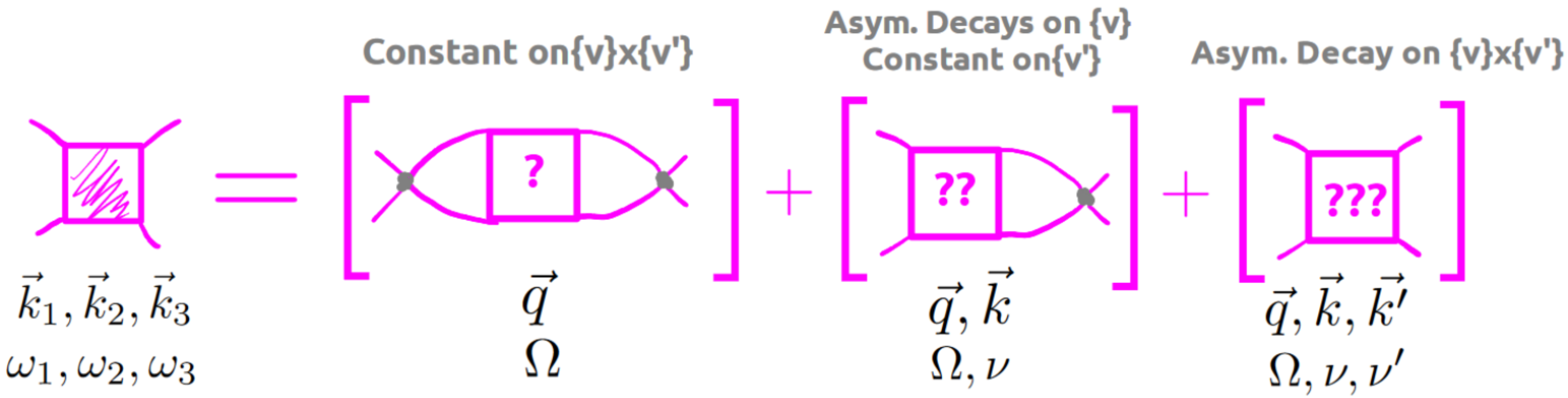
Husemann et al (2012)

Frequency Asymptotics

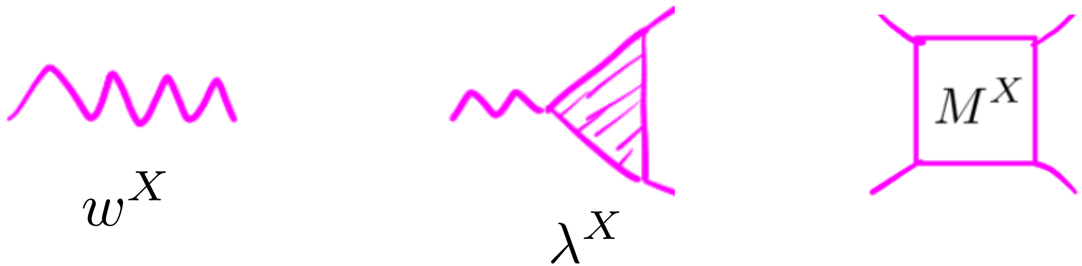
G. Rohringer (dissertation), N. Wentzell et al (2020)

Dependence on fermionic frequencies enter only through $G(\omega) \sim \omega^{-1}$

$\rightsquigarrow$ **Isolate fermionic frequency dependence from the bosonic and treat fermionic only on a small finite interval**



Note: SBE quantities fall naturally under this classification!



At large frequencies, they decay to their static bare values.

SBE approximations

P. Bonetti et al (2022)
K. Fraboulet, S. Heinzelman et al (2022)
M. Gievers et al (2022)

"Neglect multi-boson exchanges M^X"

Two Ways:

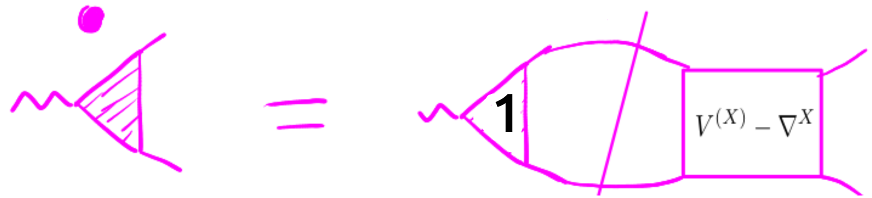
before taking derivative
"SBEb approximation"

or

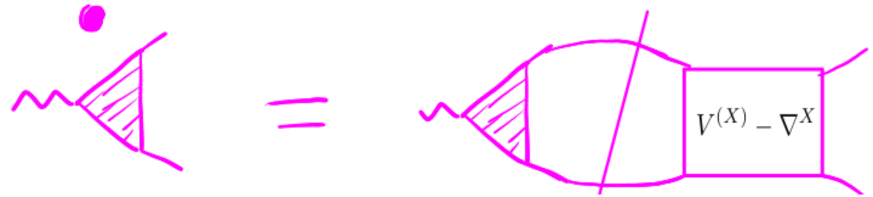
after taking derivative
"SBEa approximation"

Different equations!
E.g.

SBEb $\quad \partial_t \lambda_k^X(q) \;\hat{=}$



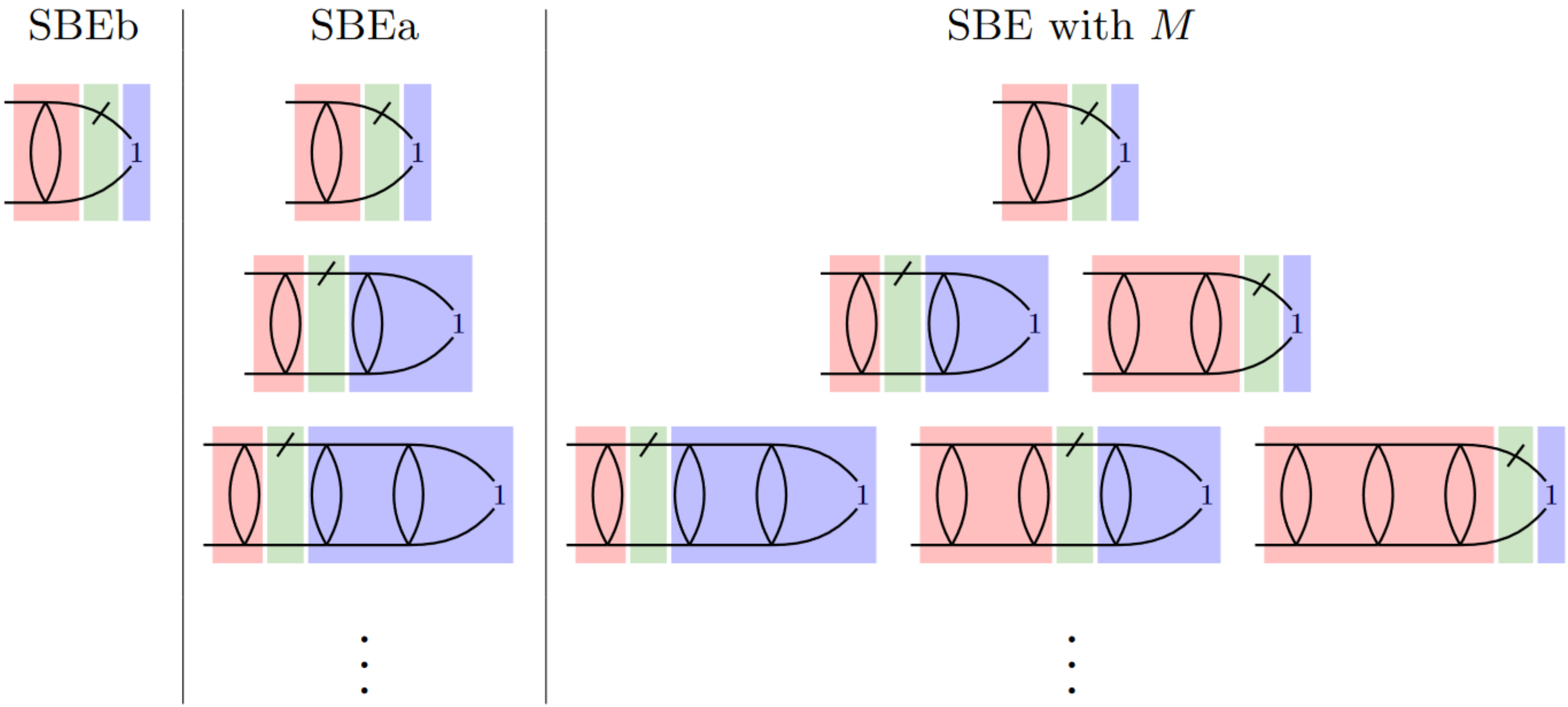
SBEa $\quad \partial_t \lambda_k^X(q) \;\hat{=}$



SBE approximations Comparison

Schematic of diagrams generated for flow of λ^X

Row n = diagrams now present due to step n



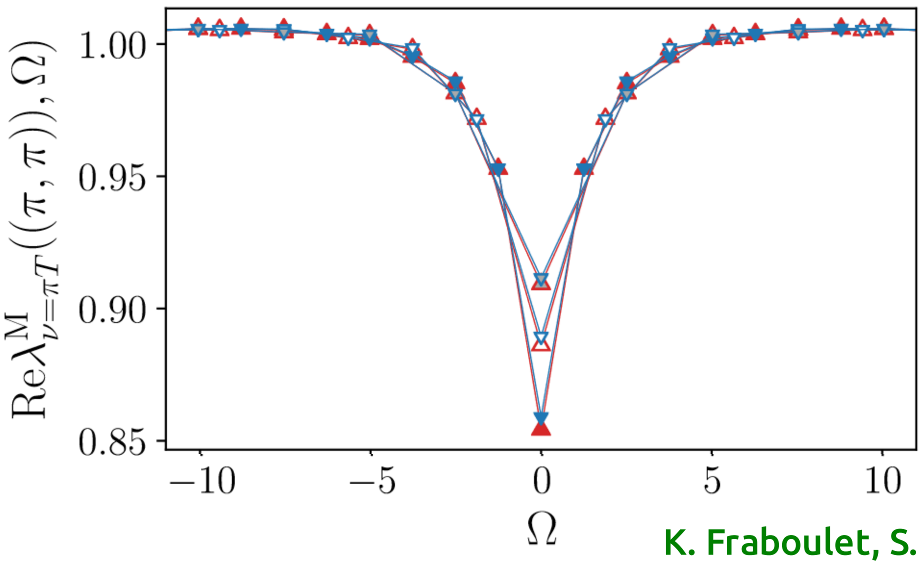
K. Fraboulet, S. Heinzelman et al (2022)

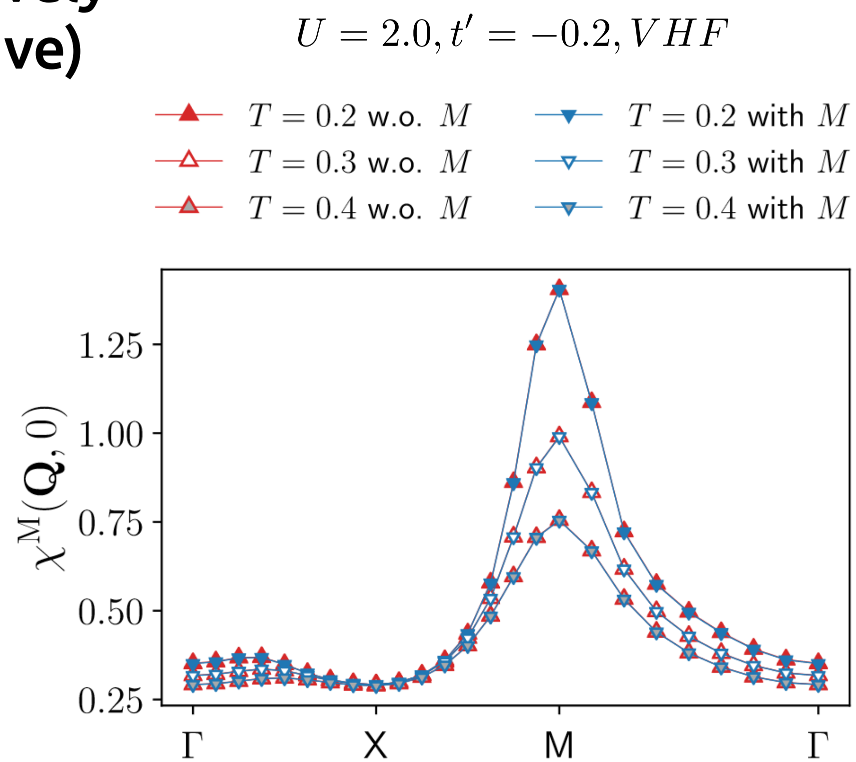
SBE Approximations Performance

SBEb -> No good..

SBEa -> very successful, even quantitatively
(at transition, only qualitative)

example plots (square lattice)





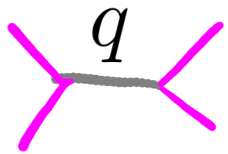
K. Fraboulet, S. Heinzelman et al (2022)

Huge reduction of numerical effort

Extended Interactions: Challenges

Non-local bare interactions:

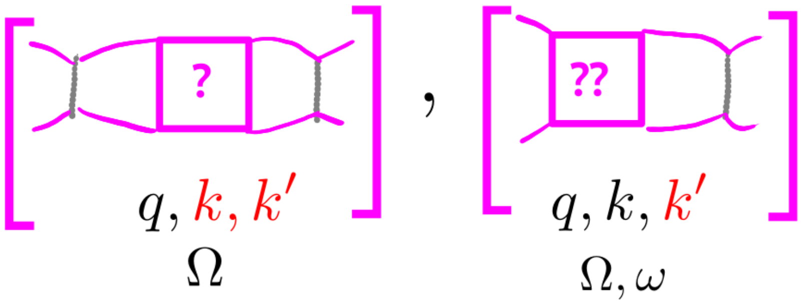
$$V_0 = U\delta(\sum k_i = 0) + W(k_1 - k_2) \hat{=}$$



Attempts to apply bona fide SBE with V_0 - reducibility yields....

Challenges

- $w^X(q) \rightsquigarrow w^X(q, k)$ not any more purely Bosonic
- Frequency asymptotics



Inefficient!

- High momentum dependence is needed (form factors) to capture the extended interaction, even for s-wave physics!

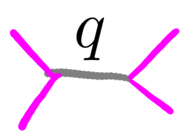
Rethinking SBE

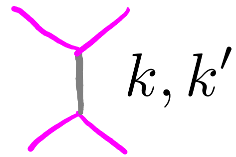
SBE = Single **Boson** Exchange

Must retain the pure bosonic dependence of w^X

- **In the parametrisation of each channel, we split:**

$$V_0^{(X)}(k_1, k_2, k_3) = V^X_{0,bos}(q) + V^X_{0,ferm}(k, k')$$





(bare interaction included)

- **Classify the diagrams in terms of $V_{0,bos}^{(X)}$ reducibility**

Extended SBE

- $V_{0,bos}^{(X)}$ now plays the role of the bare interaction in each channel.
- $V_{0,ferm}^{(X)}$ pushed to the rest function.

$\rightsquigarrow w(q)$ retains its pure bosonic momentum dependence!

- **New initial conditions:**

$$w_{t=0}^{X} = V_{0,bos}^{X}, \quad M_{t=0}^{X} = V_{0,ferm}^{X}, \quad \lambda_{t=0}^{X} = 1 \text{ if s-wave, else } 0$$

- **Technical results:**

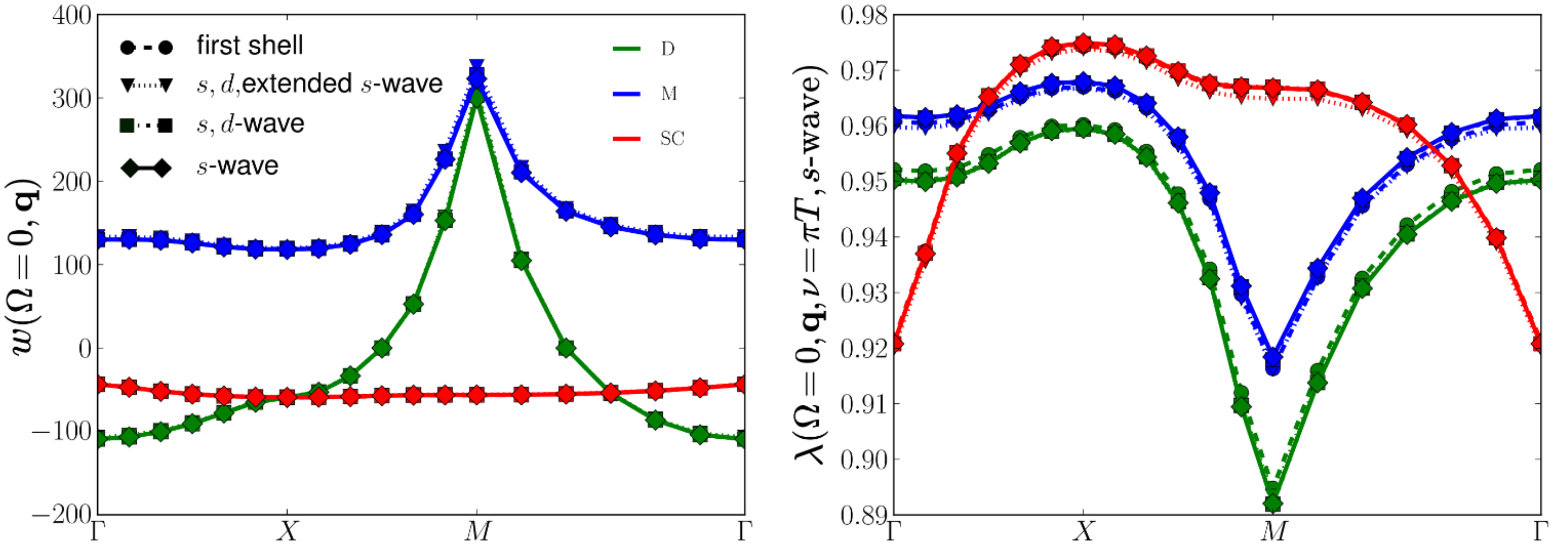
  - For "s-wave orders", the multiboson exchange contributions are negligible (SBEa)
  - Non-local form factors not needed
  - The asymptotic objects for M and lambda are negligible.

Technical Results: Form Factors

$U = 2, W = 0.5$

$T = 0.2$

(obtained by S. Heinzelman on the square lattice)

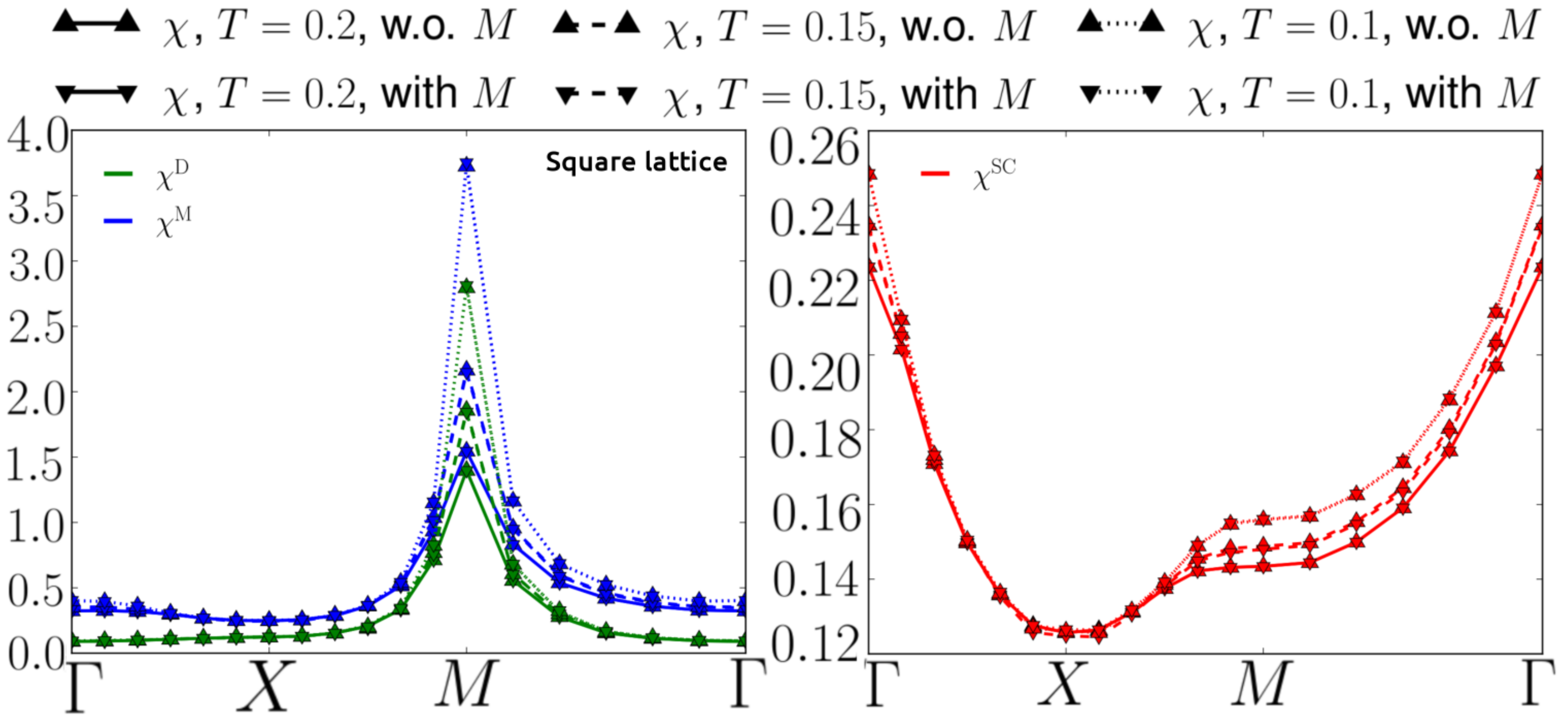


Reasonings:

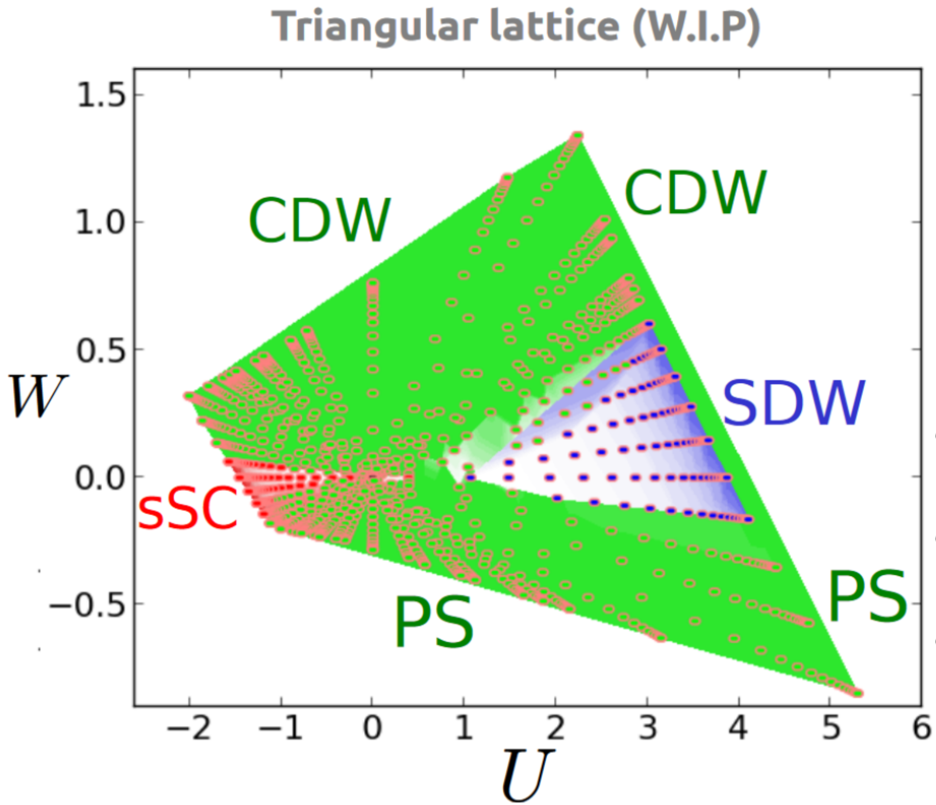
- Mixed bubbles vanish
- Hedin vertex is zero at the start of the flow

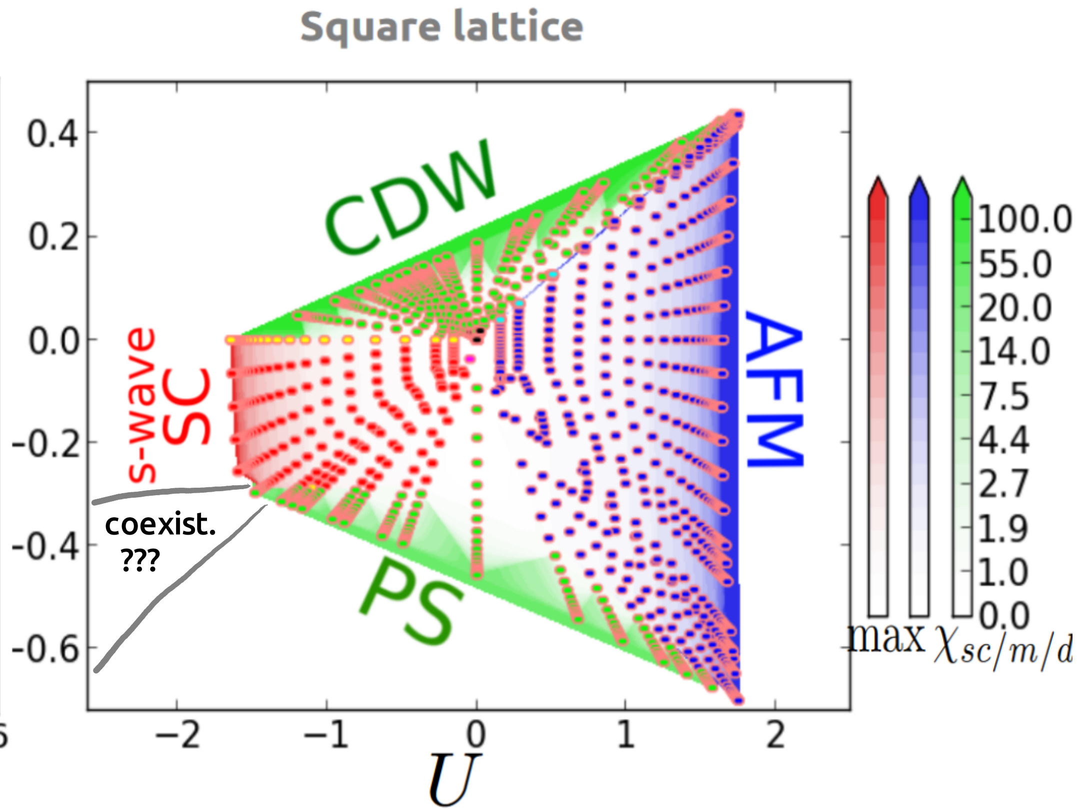
Technical Results: SBEa

$U = 2, W = 0.5$ (obtained by S. Heinzelman)



Phase Diagrams (SBEa)





- Square lattice: Agreement with other methods in CDW to AFM transition.
  Agreement with E. Linner et al (2023) in the attractive regime (Fluctuating field method)

SBE via Partial Bosonisation

T. Denz et al (2019)

Alternative way to derive the SBE equations

$$V_0 = (V_0 + V_0 + V_0) - 2V_0 \quad \rightsquigarrow$$

Hubbard-Stratanovich transform each term in the bracket for each of the three channels

$\rightsquigarrow$ **fRG on** $S_{bos}[\bar{\psi}, \psi, \vec{\phi}_m, \phi_d, \phi_{sc}, \phi^*_{sc}]$

with regulator only on fermionic part

As a matter of fact, we can formulate extended SBE also in this language:

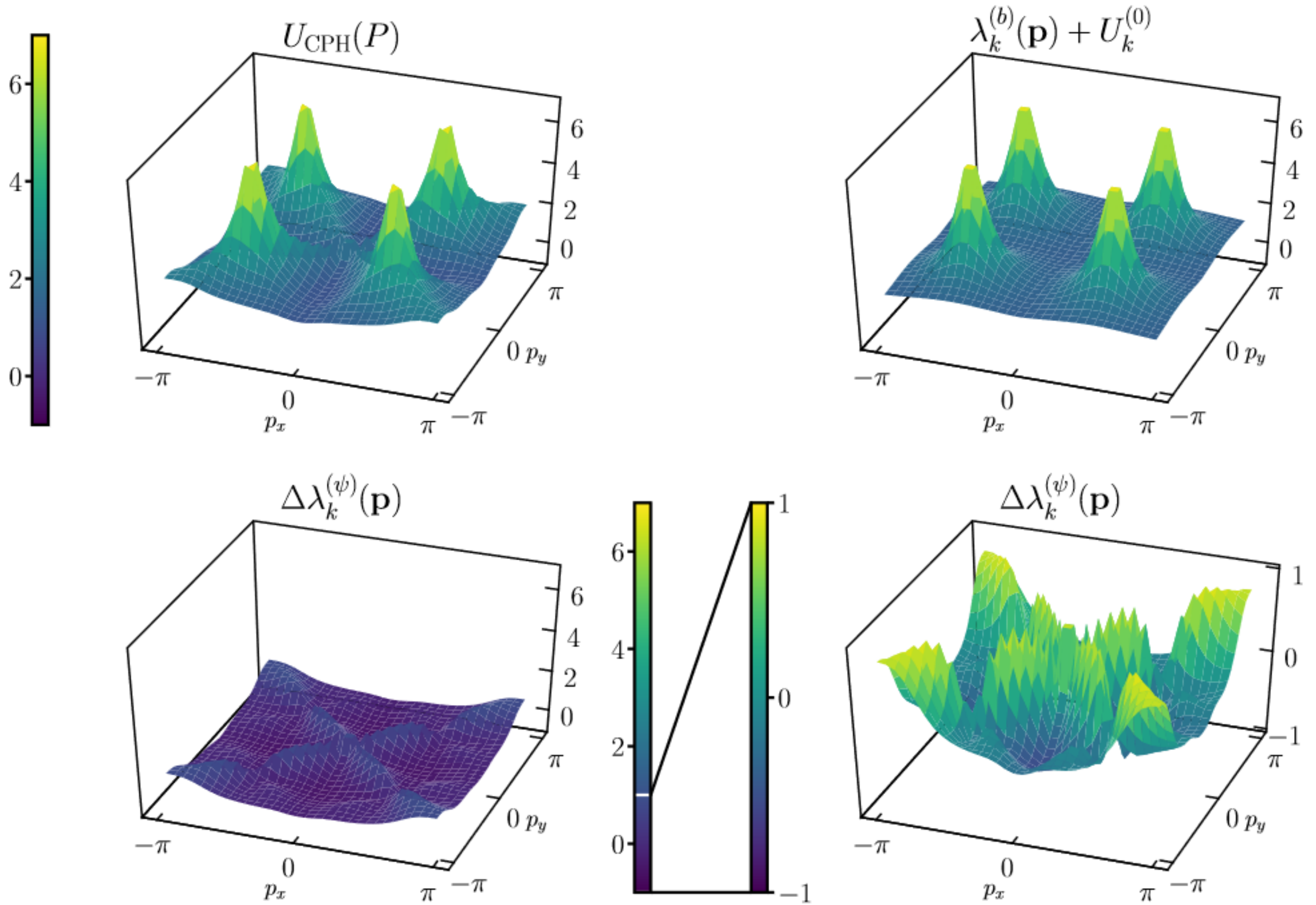
$$V_0 = \sum_X (V^X_{0,bos}) + \sum_X (V^X_{0,ferm}) - 2V_0$$

Fierz ambiguity problem:

Multitude of ways to do this splitting! Upon truncation -> Potential bias!

SBEa approximation (pretty much)

T. Denz et al (2019)



Fierz Ambiguity

Table reported:

"bias free"

"pure fermionic"

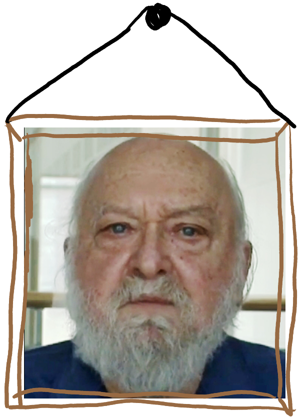
	SSB	FM	FL	BF
PF		✓		✓
HS	✓			✓
DB	✓		✓	
DBF	✓	✓	✓	✓

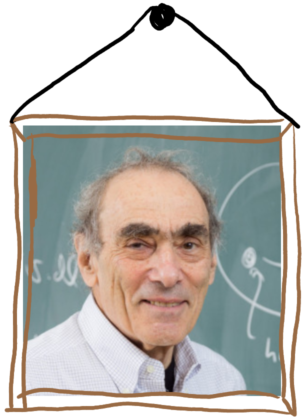
But we know from the SBE point of view that the two are equivalently bias-free!

T. Denz et al (2019)

"Dichotomy of Approximations"

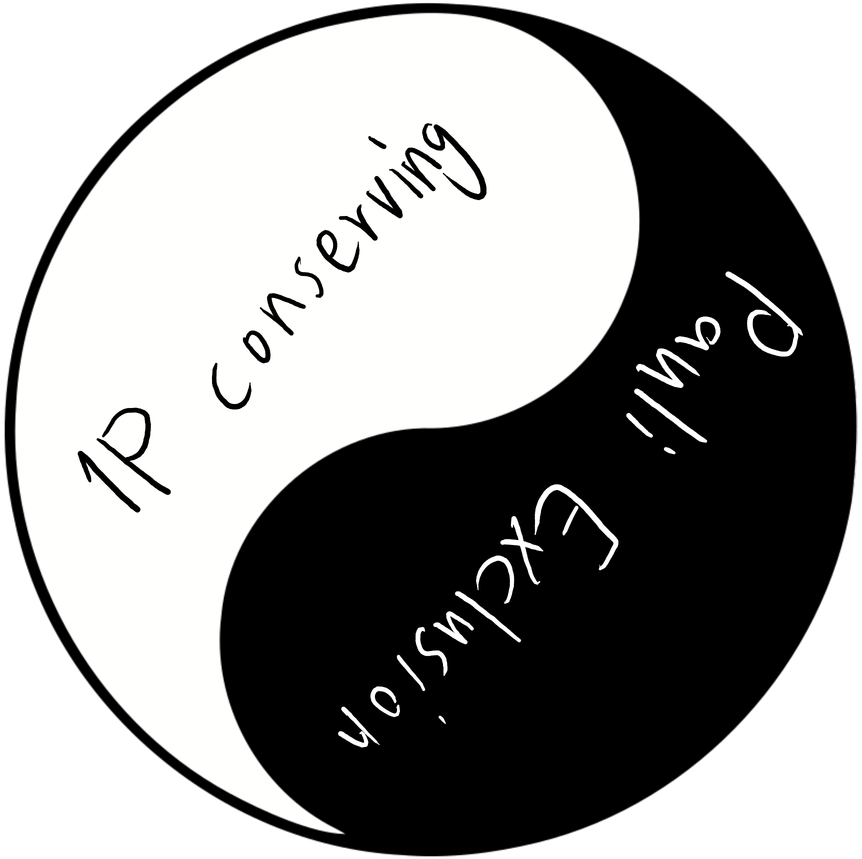
R. A. Smith (1991)

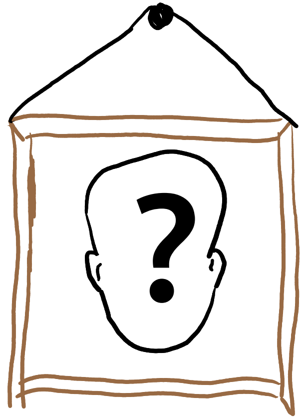




L. Kadanoff and G. Baym(1961)

Φ -derivable approximations





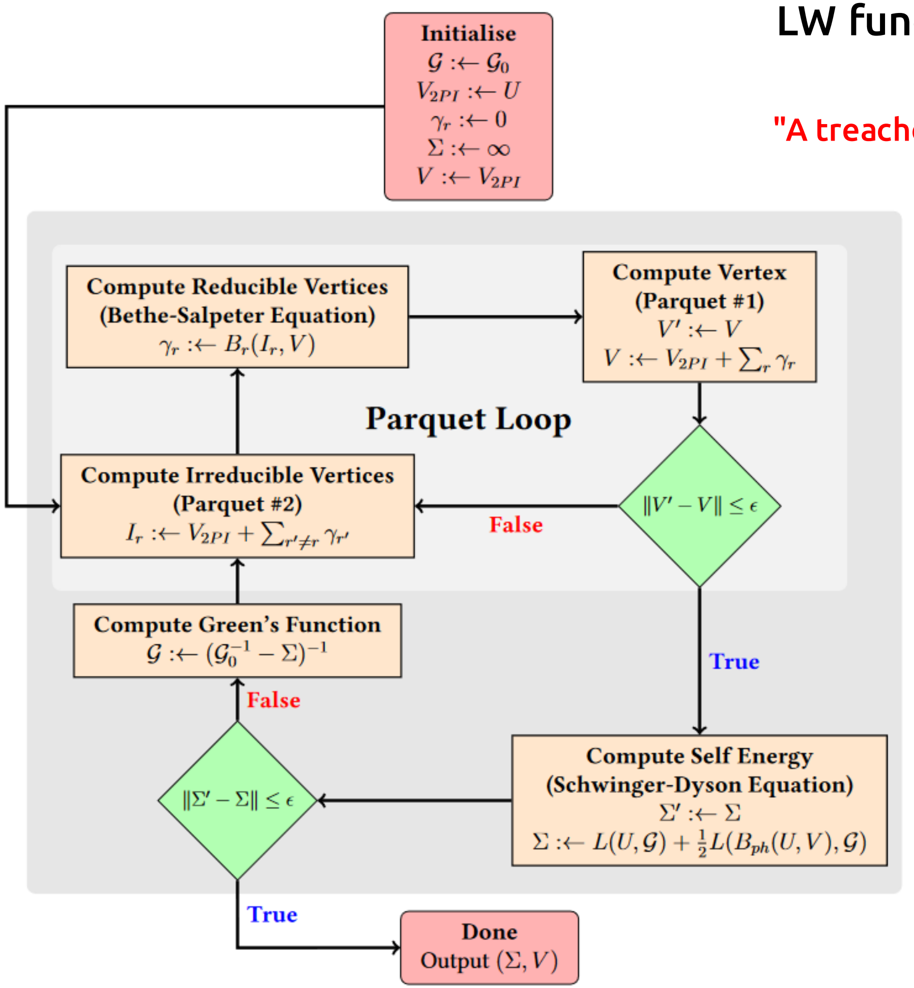
C. De Dominicis and P. C. Martin (1964)

Parquet Formalism

Thm (Smith): Both $\Longrightarrow$ Exact solution

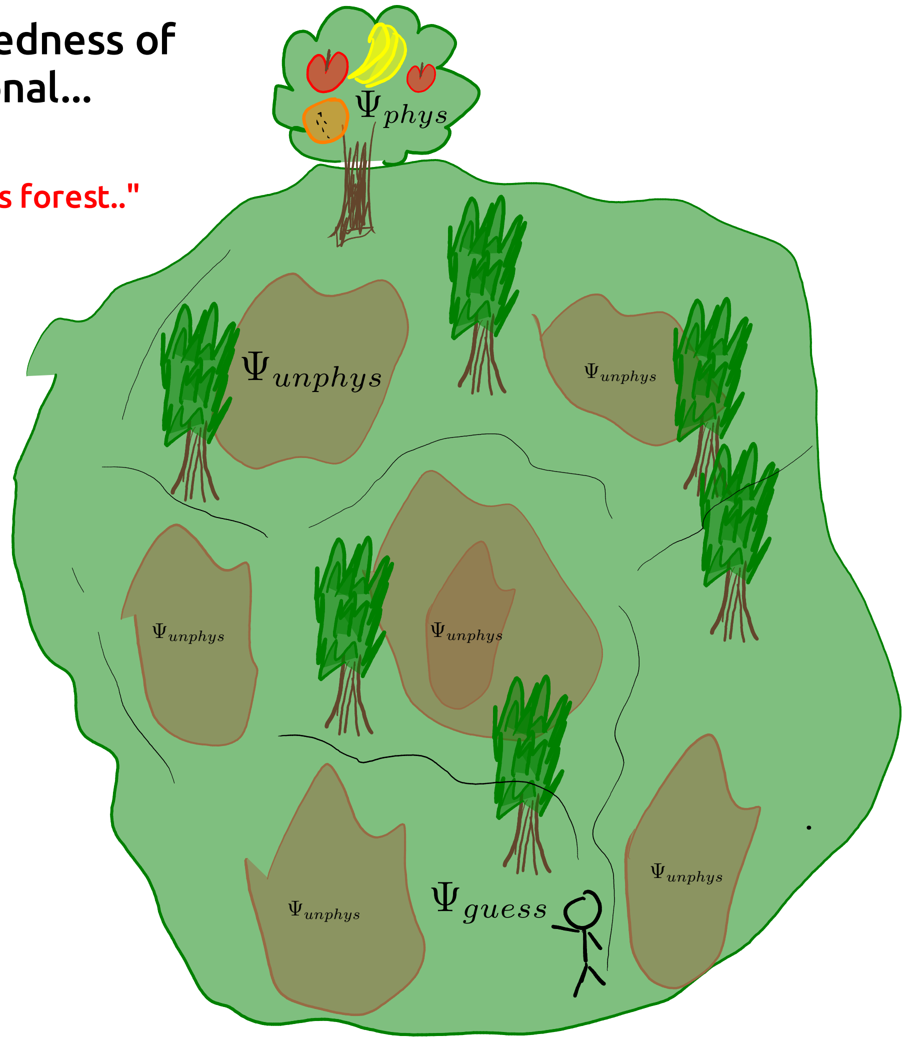
Pauli Preserving Many Body Approximations

Example: Parquet Formalism



Multi-valuedness of LW functional...

"A treacherous forest.."



Multiloop Extension

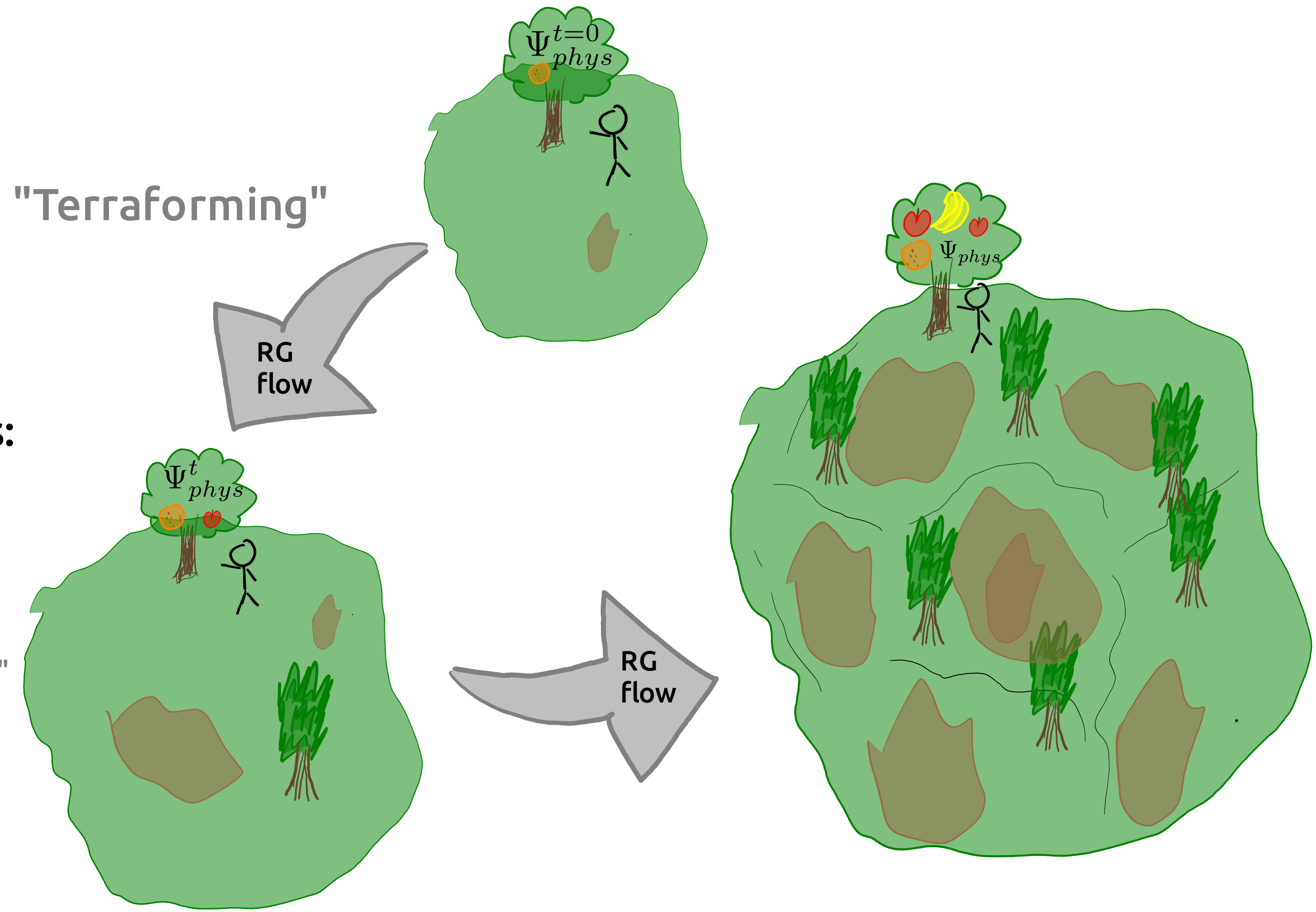
F. Kugler and J. von Delft (2018)

Low finite temperatures

more unphysical sinks,
difficulty to converge.

Multiloop flow equations:

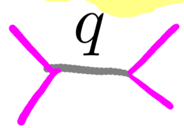
- flow equations for "corrections" to the state such that when converged -> Parquet
- Promise in avoiding unphysical solutions (given "good" frequency treatment).
- Preliminary results (collab with: K. Fraboulet): SBEa approximation works well at 2-loop level!

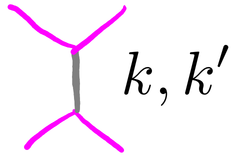


Conclusion

SBE with

$$V_0^{(X)}(k_1, k_2, k_3) = V_{0,bos}^X(q) + V_{0,ferm}^X(k, k')$$





(bare interaction included)

Very efficient approximation scheme!

- SBEa approximation: no flow for M^X
- Reduction in number of form factors
- No extra asymptotics.
- Shows promise in exploring new grounds quantitatively.