Self-consistent two-particle calculations with quantics tensor trains – solving the parquet equations

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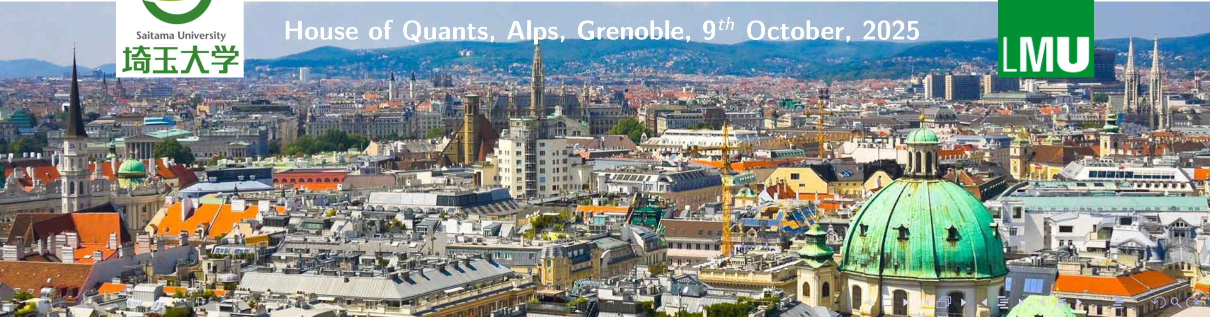
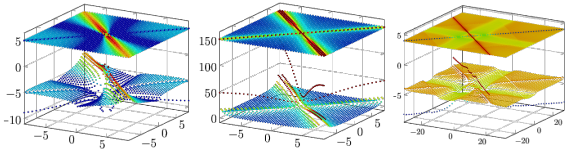
House of Quants, Alps, Grenoble, 9th October, 2025



Outline

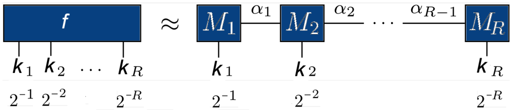
Motivation

- Two-particle vertex function
- Parquet equations
- Challenges



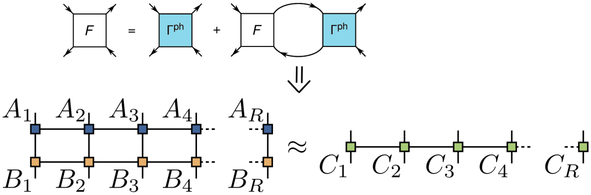
Dimensional reduction

- Compressibility of vertices
- Quantics tensor trains (QTTs)
- Learning the QTT with TCI



Parquet equations with QTTs

- Equations –> contractions of tensors
- Performance and scaling
  S. Rohshap et al PRR 7, 023087 (2025)
- Outlook:
  momentum and orbital dependence



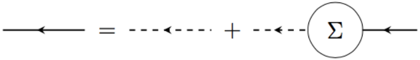
One-particle and two-particle response functions

One-particle response

- Electronic spectra given by the one-particle Green's function

$$G_{\alpha\lambda}(\vec{k},\nu) = -\int_0^\beta d\tau e^{i\nu\tau}\langle T_\tau \hat{c}_{\vec{k}\alpha}(\tau)\hat{c}^\dagger_{\vec{k}\lambda}(0)\rangle$$

- Dyson equation: $G = G_0 + G_0 \Sigma G$



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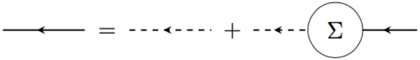
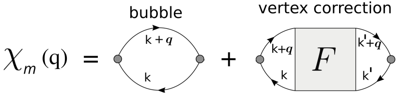
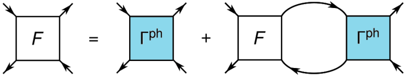


Two-particle response

- Magnetic susceptibility $\chi_m = \frac{\partial M}{\partial H}$ contains two-particle vertex



- Bethe-Salpeter equation



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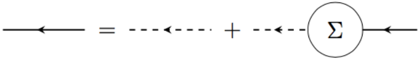

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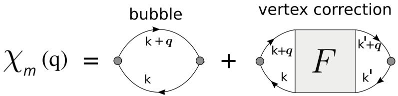

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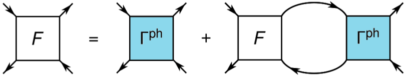
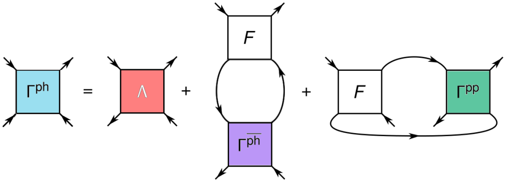


- Parquet equation



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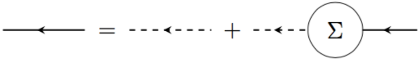
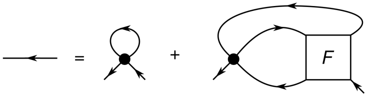


- Schwinger-Dyson equation



C. DeDominicis, P.C. Martin, J.Math.Phys. 5, 31 (1964),
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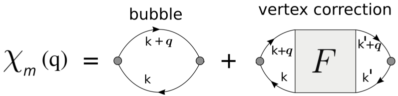

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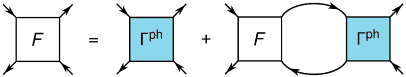

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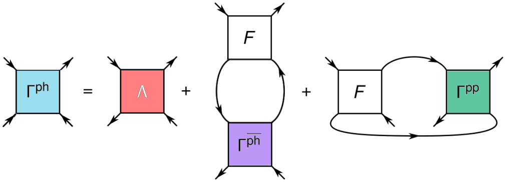
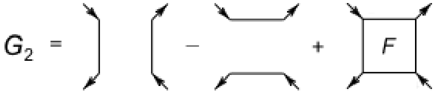


What is a two-particle vertex?

- Connected part of the two-particle Green's function

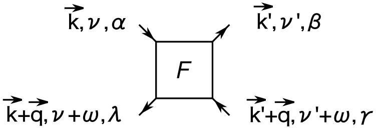
$$G_2 = \langle T_\tau \hat{c}_{\vec{k}\alpha}(\tau_1)\hat{c}^\dagger_{\vec{k}+\vec{q}\lambda}(\tau_2)\hat{c}_{\vec{k}'+\vec{q}\gamma}(\tau_3)\hat{c}^\dagger_{\vec{k}'\beta}(0)\rangle$$



- Describes all scattering processes between two particles or a particle and a hole (in a solid)
- Multivariate function

$$F_{\alpha\lambda\gamma\beta}(\vec{k},\nu,\vec{k}',\nu',\vec{q},\omega)$$

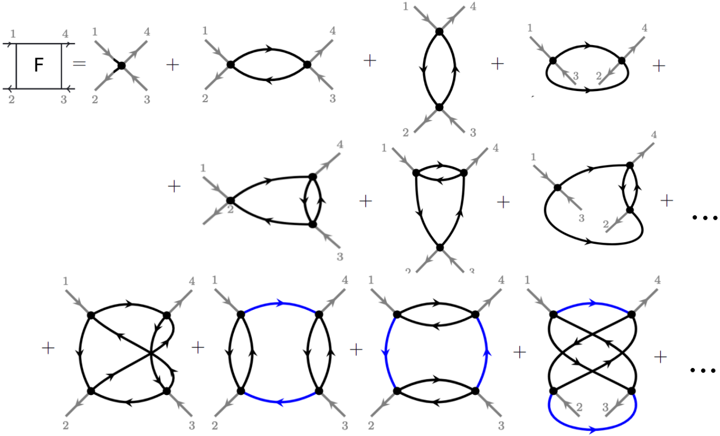
  dependent on 4 spin-orbital indices, 3 momenta and 3 frequencies



- Memory: 1 orbital, 80 frequencies and 56×56 momentum slices (2D) need 240 Petabytes!

What is in a two-particle vertex?

Expansion of F



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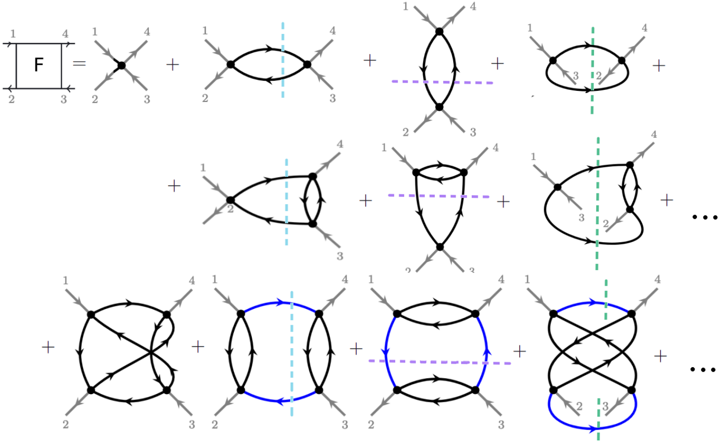

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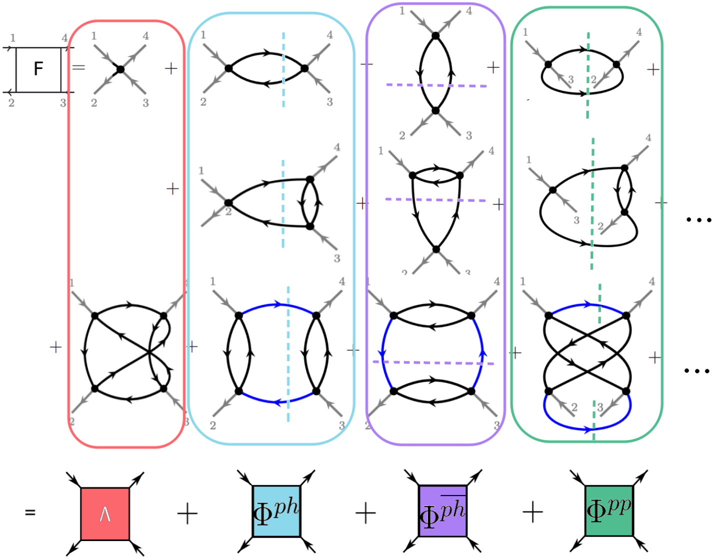
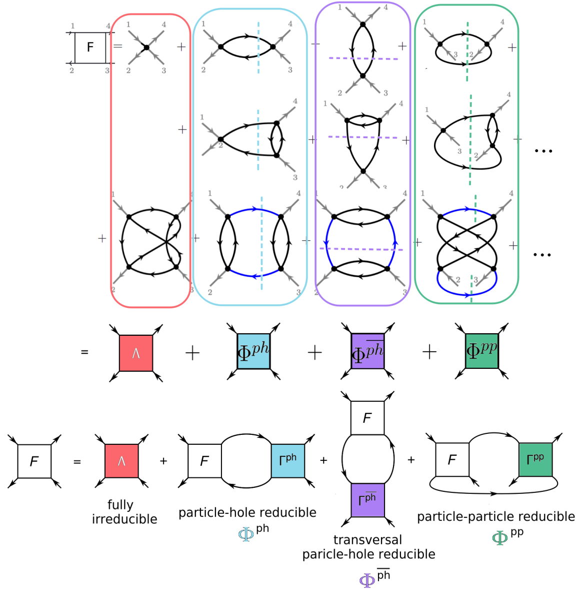
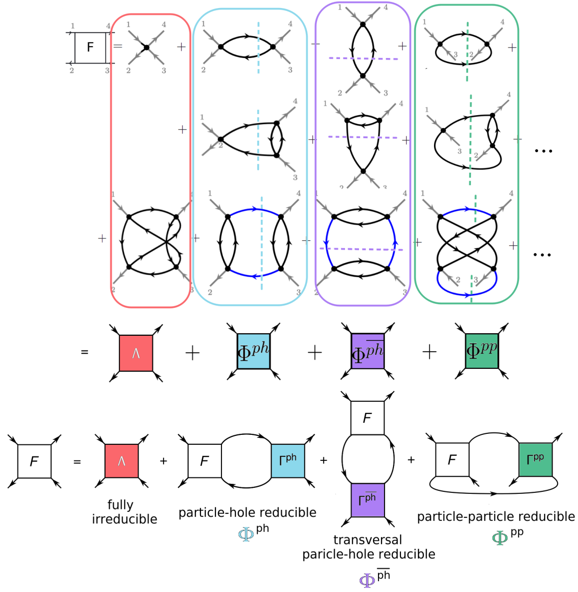


Classification of two-particle diagrams



Classification of two-particle diagrams —> parquet equations



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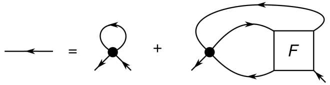
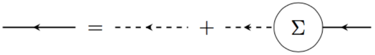


- Dyson equation: $G = G_0 + G_0 \Sigma G$



- Input: Fully irreducible vertex Λ (approximated) and non-interacting Green's function G_0

C. DeDominicis, P.C. Martin, J.Math.Phys. 5, 31 (1964),
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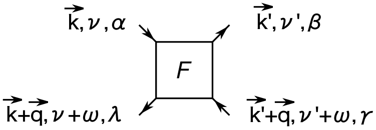
- Describes all scattering processes between two particles or a particle and a hole (in a solid)
- Multivariate function

$$F_{\alpha\lambda\gamma\beta}(\vec{k},\nu,\vec{k'},\nu',\vec{q},\omega)$$

dependent on 4 spin-orbital indices, 3 momenta and 3 frequencies



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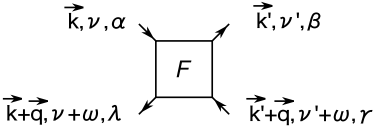

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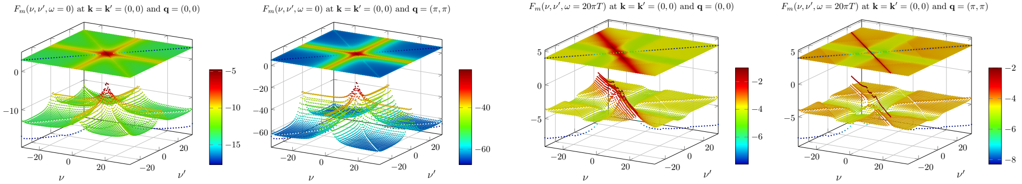


G. Li, AK, P. Pudleiner, K. Held, Comp. Phys. Comm. 241, 146–154 (2019)

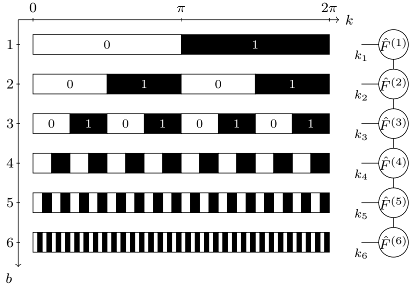
Quantics representation of functions

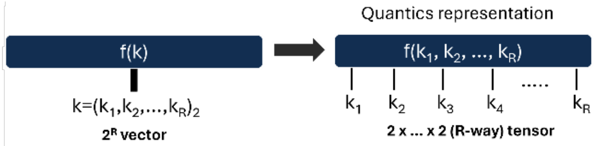
- The argument k of a function $f(k)$ is rewritten in a binary representation

$$f(k) = f((k_1 \dots k_R)_2) = f(k_1, k_2, \dots, k_R)$$

- E.g. for momentum we can have

$$k = 2\pi(k_1 \dots k_R)_2 = k_1\pi + k_2\frac{\pi}{2} + \dots + k_R\frac{2\pi}{2^{-R}}$$





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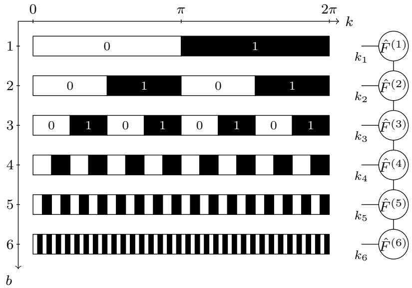
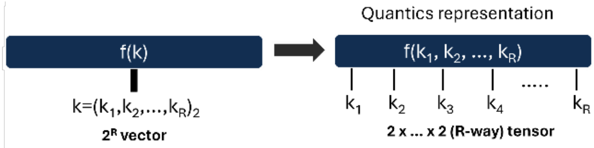
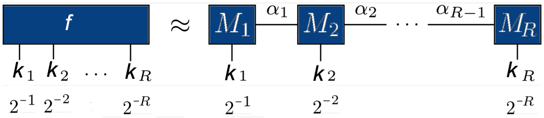




- Tensor train representation (MPS): R three-way tensors

$$f(k_1, \dots, k_R) \approx \sum_{\alpha_1=1}^{D_1} \cdots \sum_{\alpha_{R-1}=1}^{D_{R-1}} [M_1]^{k_1}_{1\alpha_1} \cdots [M_R]^{k_R}_{\alpha_{R-1}1}$$



- The level of compression depends on bond dimensions D_l

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Two-particle vertices in QTT representation

- QTT for frequency dependence (discrete Matsubara frequencies)

$$F(\nu,\nu',\omega) = F((\nu_1\dots\nu_R)_2,(\nu'_1\dots\nu'_R)_2,(\omega_1\dots\omega_R)_2)$$
$$= F(\nu_1,\nu'_1,\omega_1,\nu_2,\nu'_2,\omega_2,\dots,\nu_R,\nu'_R,\omega_R)$$

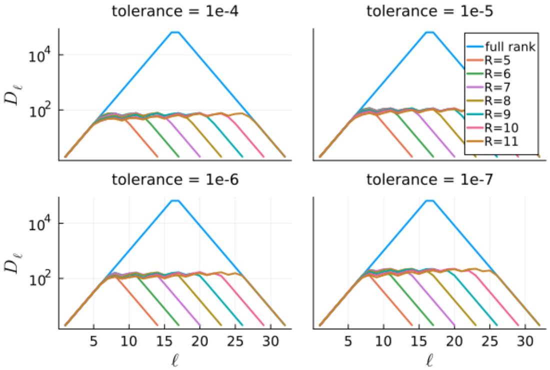
- Arguments are regrouped to put the same scales together (interleaved representation)

$$F \approx \prod_{\ell=1}^{3R} M_\ell = \sum_{\alpha_\ell}^{D_\ell} [M_1]^{\nu_1}_{1\alpha_1}[M_2]^{\nu'_1}_{\alpha_1\alpha_2}\cdots[M_L]^{\omega_R}_{\alpha_{L-1}1}$$

S. Rohshap et al, PRR 7, 023087 (2025)
Y. Núñez Fernández et al, PRX 12, 041018, (2022)
M. Ritter et al, PRL 132, 056501 (2024)
Y. Núñez Fernández et al, SciPost Phys. 18, 104 (2025)

- Bond dimensions D_ℓ of QTT of the full two-particle vertex F obtained with TCI at different tolerances for Hubbard atom

$$\hat{\mathcal{H}} = U\hat{n}_\uparrow\hat{n}_\downarrow - \mu(\hat{n}_\uparrow + \hat{n}_\downarrow)$$



Full set of parquet equations:

- Parquet equation (elementwise sum with shifts of variables)

$$F^{\nu\nu'\omega} = \Lambda^{\nu\nu'\omega} + \Phi_{ph}^{\nu\nu'\omega} + \Phi_{\overline{ph}}^{\nu(\nu+\omega)(\nu'-\nu)} + \Phi_{pp}^{\nu\nu'(\nu+\nu'+\omega)}$$

- Bethe-Salpeter equation (convolution/matrix multiplication)

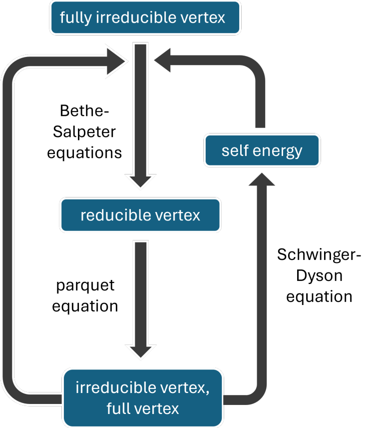
$$\Phi_r = \Gamma_r (GG)_r F \quad \text{with} \quad \Gamma_r = F - \Phi_r$$

- Schwinger-Dyson equation

$$\Sigma = \Sigma_{HF} + U\ GGG\ F$$

  and Dyson equation $G = [G_0^{-1} - \Sigma]^{-1}$

- Input: Fully irreducible vertex Λ (approximated) and non-interacting Green's function G_0



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C. Eckhardt, C. Honerkamp, K. Held, and AK, PRB 101, 155104 (2020)
F. Krien, AK, and K. Held, PRR 3, 013149 (2021), F. Krien, AK, EPJB 95, 69 (2022)
J-M. Lihm, S.-S.B. Lee, D. Kiese, F. Kugler, arXiv:2505.20116 (2025)

Parquet equations as operations on tensor trains

- Parquet equation (elementwise sum with shifts of variables)

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

- Bethe-Salpeter equation (BSE) (convolution/matrix multiplication)

$$\Phi_r \;=\; \Gamma_r \chi_0 F$$

- Schwinger-Dyson equation (SDE)

$$\Sigma = \; \Sigma_{HF} + U \; GGG \; F$$

and Dyson equation $G = [G_0^{-1} - \Sigma]^{-1}$

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- Channel transformation (affine transformation)

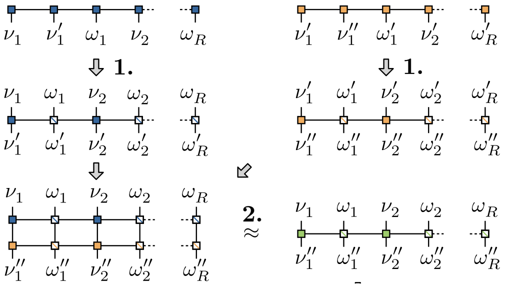
$$\Phi_{ph}^{\nu\nu'\omega} \rightarrow \Phi_{ph}^{\nu(\nu+\omega)(\nu'-\nu)}$$

MPO-MPS contraction

- Matrix multiplication

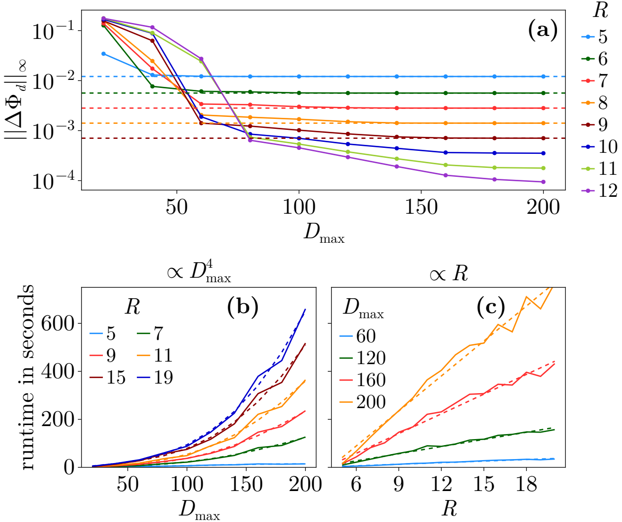
$$\Phi_{ph}^{\nu\nu'\omega} = \sum_{\nu_1\nu_2} \Gamma_{ph}^{\nu\nu_1\omega} \chi_0^{\nu_1\nu_2\omega} F^{\nu_2\nu'\omega}$$

MPO-MPO contractions

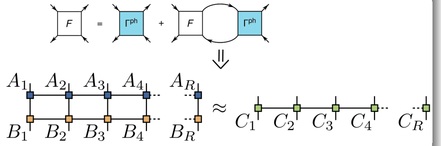


Test case: Hubbard atom $\hat{\mathcal{H}} = U\hat{n}_\uparrow\hat{n}_\downarrow - \mu(\hat{n}_\uparrow + \hat{n}_\downarrow)$. Scaling.

$$\Phi_d^{\nu\nu'\omega} = -\sum_{\nu_1\nu_2} \Gamma_d^{\nu\nu_1\omega}\chi_0^{\nu_1\nu_2\omega}F_d^{\nu_2\nu'\omega}$$



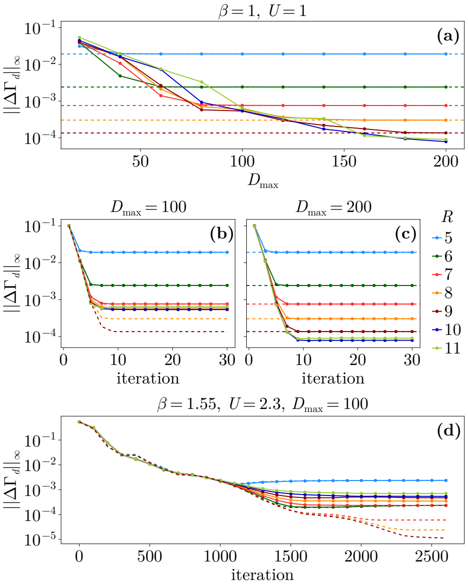
- BSE –> MPO-MPO contraction



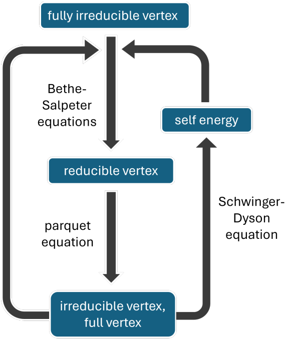
- Error $\Delta\Phi_d = \Phi_d - \Phi_{d\,exact}$ decays exponentially in D_{max}
- $\mathcal{O}(D_{max}^4 R)$ runtime scaling
- Runtime linear in R (i.e. only logarithmic in grid size 2^R !)
- Comparison to exact vertices here (analytically known for atom)
- The same scaling for Anderson impurity model

S. Rohshap et al, PRR 7, 023087 (2025)

Test case: Hubbard atom $\hat{\mathcal{H}} = U\hat{n}_\uparrow \hat{n}_\downarrow - \mu(\hat{n}_\uparrow + \hat{n}_\downarrow)$. Self-consistency.



Full iterative parquet scheme

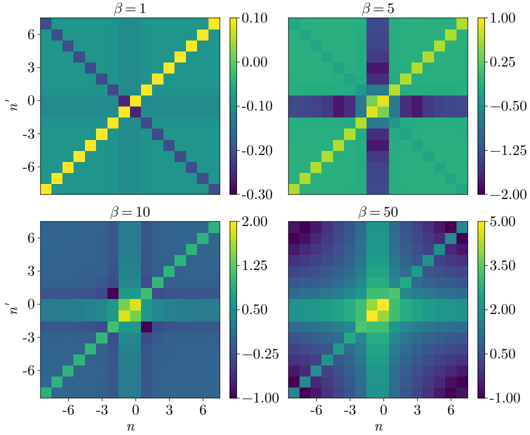


- For $\beta = 1,\ U = 1$ fast convergence, no error accumulation
- For $\beta = 1.55,\ U = 2.3$ slow convergence (as expected, very close to divergence of Γ_d)

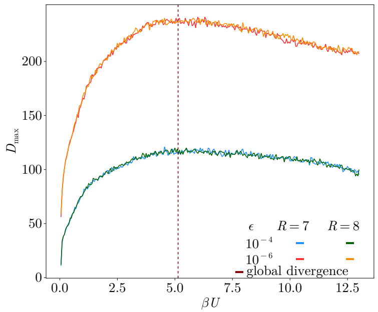
$$||\Delta\Gamma_d||_\infty := \frac{||\Gamma_{d,\text{iterative}} - \Gamma_{d,\text{exact}}||_\infty}{||\Gamma_{d,\text{exact}}||_\infty}$$

Test case: Hubbard atom $\hat{\mathcal{H}} = U\hat{n}_\uparrow\hat{n}_\downarrow - \mu(\hat{n}_\uparrow + \hat{n}_\downarrow)$. Temperature dependence

- Vertex $F_d^{\nu\nu'\omega}$ at $\omega = 0$ for different temperatures $\beta = 1/T$



- Maximum bond dimension of QTT for F_d vs $\beta = 1/T$ (at $U = 1$)

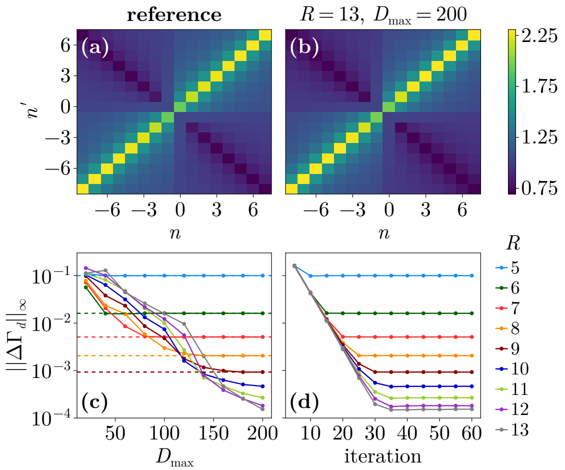


- Dashed line is at $\beta U \approx 5.14$, where Γ_d has a global divergence
- $D_{\max}$ has a broad maximum and then even decreases with β

S. Rohshap et al, PRR 7, 023087 (2025)

Single impurity Anderson model at weak coupling

Irreducible vertex Γ_d at $\beta = 10,\ U = 1$



Model: impurity coupled to bath electrons

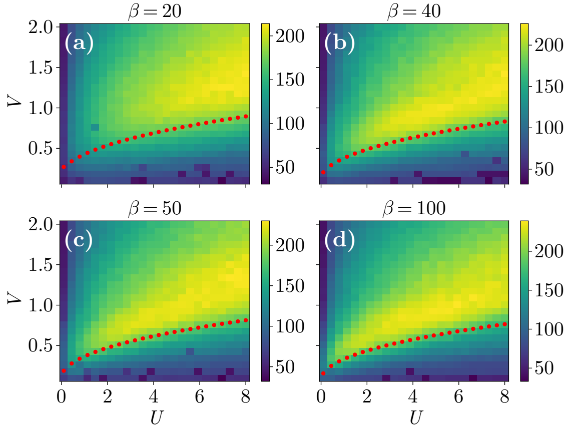
$$\hat{\mathcal{H}} = U\hat{n}_{d,\uparrow}\hat{n}_{d,\downarrow} + \varepsilon_d(\hat{n}_{d,\uparrow} + \hat{n}_{d,\downarrow}) + \sum_{\mathrm{k}\sigma} \varepsilon_{\mathrm{k}} \hat{c}^\dagger_{\mathrm{k},\sigma}\hat{c}_{\mathrm{k},\sigma} + \sum_{\mathrm{k}\sigma}\left(V_{\mathrm{k}}\hat{c}^\dagger_{\mathrm{k},\sigma}\hat{d}_\sigma + V^*_{\mathrm{k}}\hat{d}^\dagger_\sigma\hat{c}_{\mathrm{k},\sigma}\right)$$

- Flat bath density of states $\rho(\epsilon) = \theta(D - |\epsilon|)/(2D)$ with $D = 10$
- $V_{\mathrm{k}} = V = 2$, $\varepsilon_d = -U/2$
- Parquet approximation $\Lambda = U$ valid for weak to intermediate coupling
- Reference data from equidistant grid calculations with smart treatment of high frequency parts (multi-boson exchange formulation)
- Exponential scaling of error with D_{max}
- Runtime scaling $\mathcal{O}(D^4_{max}R)$

S. Rohshap et al, PRR 7, 023087 (2025)

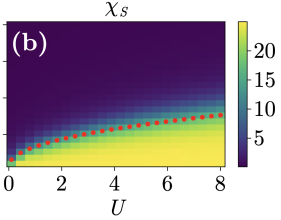
Single impurity Anderson model in the Kondo temperature regime (exact diagonalization)

$D_{\max}$ of the QTT for two-particle Green's function $G_{\mathrm{imp}}^{\uparrow\uparrow\uparrow\uparrow}$ of the impurity (from ED, fitted with TCI at tol 10^{-5})



$$\hat{\mathcal{H}} = U\hat{n}_{d,\uparrow}\hat{n}_{d,\downarrow} + \varepsilon_d(\hat{n}_{d,\uparrow} + \hat{n}_{d,\downarrow}) + \sum_{\mathrm{k}\sigma} \varepsilon_{\mathrm{k}} \hat{c}^\dagger_{\mathrm{k},\sigma}\hat{c}_{\mathrm{k},\sigma} + \sum_{\mathrm{k}\sigma}\left(V_{\mathrm{k}}\hat{c}^\dagger_{\mathrm{k},\sigma}\hat{d}_\sigma + V^*_{\mathrm{k}}\hat{d}^\dagger_\sigma\hat{c}_{\mathrm{k},\sigma}\right)$$

- $V_{\mathrm{k}} = V$, $\varepsilon_d = -U/2$, flat bath density of states $\rho(\epsilon) = \theta(D - |\epsilon|)/(2D)$ modelled by 3 sites
- $T_K(V,U) = V\sqrt{U}e^{-\pi U/8V^2}$ (red dots) separates local moment and Kondo screening regimes in spin susceptibility χ_S



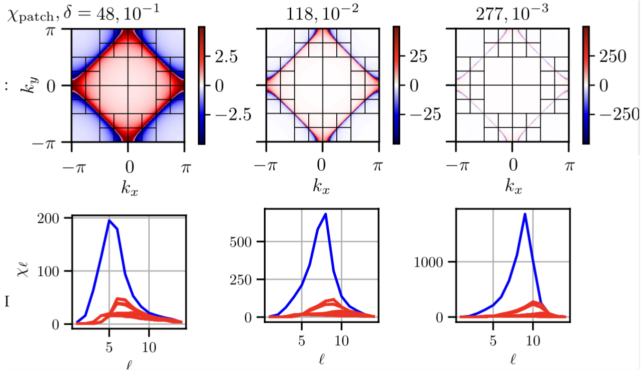
S. Rohshap, H. Ishida et al, arXiv:2507.11276

Momentum dependence

- Momentum dependence of a 2D one-particle Green's function (at a fixed $\omega + \mu$):

$$G(\mathrm{k}, \omega) = \frac{1}{\omega + \mu + 2\cos k_x + 2\cos k_y + i\delta}$$

- Bond dimension χ_l of QTCI unpatched vs patched



- Patching helps to control the bond dimension without loss in accuracy
- It allows to take advantage of sparsity
- It allows for straightforward MPI paralelization

G. Grosso et al, in preparation

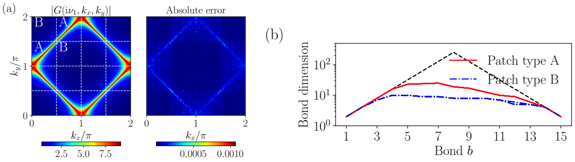
Summary and outlook

Parquet equations with QTTs

- Compression of frequency dependence with relatively low bond dimension $D \approx 100 - 200$ that seems to saturate with inverse temperature
- Equations are decomposed into MPO-MPO contractions
- Computational time scales with $\mathcal{O}(D^4 log(N_\omega))$ instead of $\mathcal{O}(N_\omega^4)$

Outlook

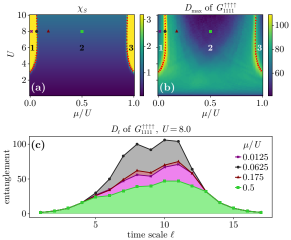
- Momentum dependence



H. Shinaoka et al, PRX 13, 021015 (2023)

G. Grosso et al, in preparation

- Bond dimension as a measure of time and length scale entanglement

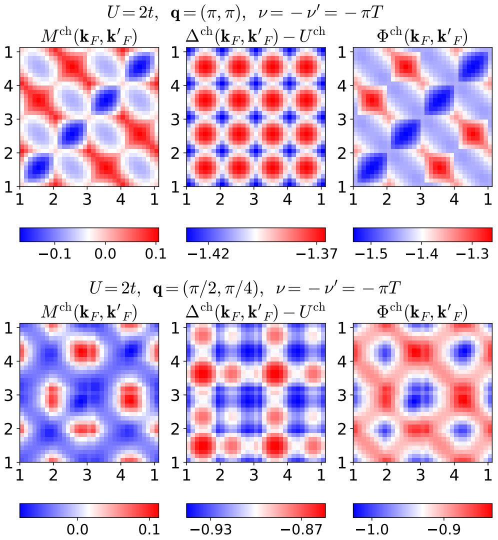


S. Rohshap et al, arXiv:2507.11276

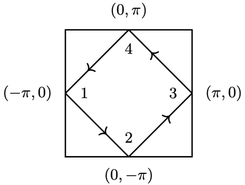
S. Rohshap et al, arXiv:2507.19069

Momentum dependence of vertices

Hubbard model on square lattice 16×16 at $\beta = 5/t$ and half-filling



- Fermionic momentum dependence along the Fermi surface



Path on the Fermi surface traversed by $\mathbf{k}_F, \mathbf{k}'_F$.

- Obtained with equidistant grid multi-boson exchange implementation on 12 nodes (512GB each), 128 cores each in $\approx$ 72 hours ($\approx 10^5$ core-h)
- Only 8 Matsubara frequencies for the core multi-boson vertex – low temperatures not possible...

F. Krien, AK, EPJB 95, 69 (2022)