Title: Learning Feynman Diagrams with Tensor Trains

Speakers: Xavier Waintal

Collection: Machine Learning for Quantum Many-Body Systems

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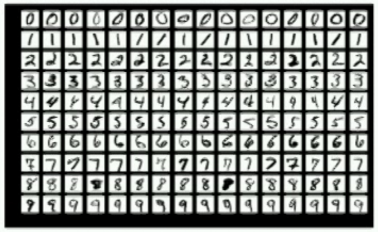
CORRELATIONS AND COMPUTATIONAL QUANTUM TRANSPORT: LEARNING FEYNMAN DIAGRAMS WITH TENSOR TRAINS

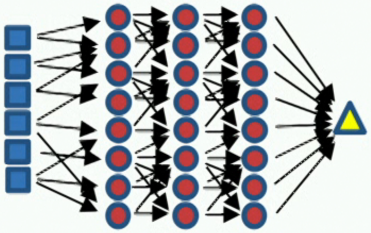
Xavier WAINTAL,
CEA Grenoble, Pheliqs IRIG
With YURIEL NUNEZ-FERNANDEZ, THOMAS KLOSS, MATTHIEU JEANNIN,CORENTIN BERTRAND, PHILIPP DUMITRESCU, Olivier Parcollet, Jason Kaye and Serge Florens.

1

Machine learning as seen by a not so expert



1) Data



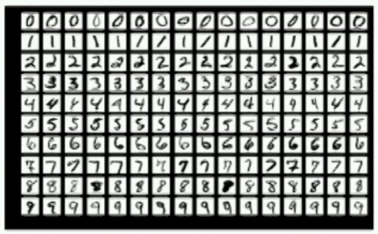
2) Model

$$C(\mu) = \frac{1}{N}\sum_{i=1}^{N}\left(y_i - f(\mu, x_i)\right)^2$$

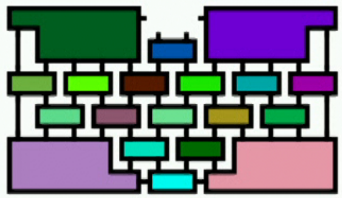
3) Cost function

4) Minimize Cost function → Enjoy

Machine learning as seen by a not so expert



1) Data



2) A highly structured model

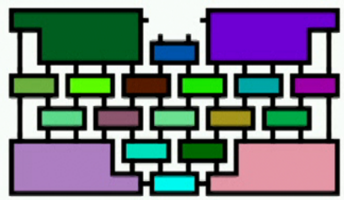
$$C(\mu) = \frac{1}{N}\sum_{i=1}^{N}\left(y_i - f(\mu, x_i)\right)^2$$

3) Cost function

4) Minimize Cost function → Enjoy

Machine learning as seen by a not so expert

$\tilde{Q}_n(v_1, \ldots, , v_n).$



$$C(\mu) = \frac{1}{N}\sum_{i=1}^{N}\left(y_i - f(\mu, x_i)\right)^2$$

~~1) Data~~ (active learning)

2) A highly structured model

3) Cost function

4) Minimize Cost function → Enjoy

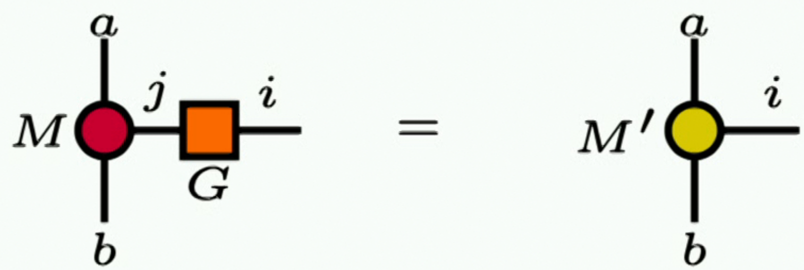
Today:

1) Tensor Trains & the Tensor Cross Interpolation (TCI) algorithm.
2) Application to the calculation of Feynman diagrams.
3) Some Kondo physics.

Oseledet
Dolgov & Savostyanov

TENSOR NETWORKS 101

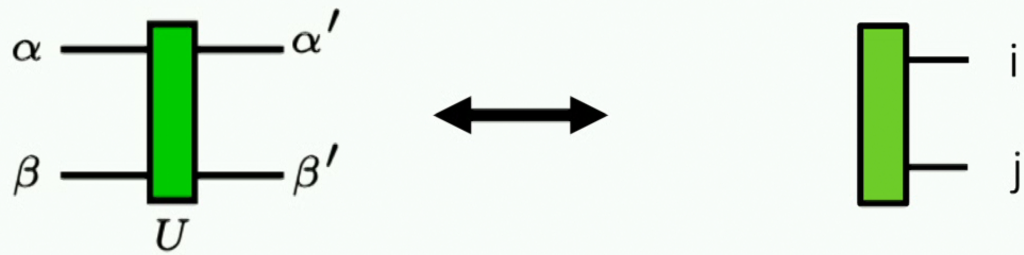
Contractions



$$M'_{abi} = \sum_j G_{ij} M_{abj}.$$

TENSOR NETWORKS 101

Grouping and degrouping of indices

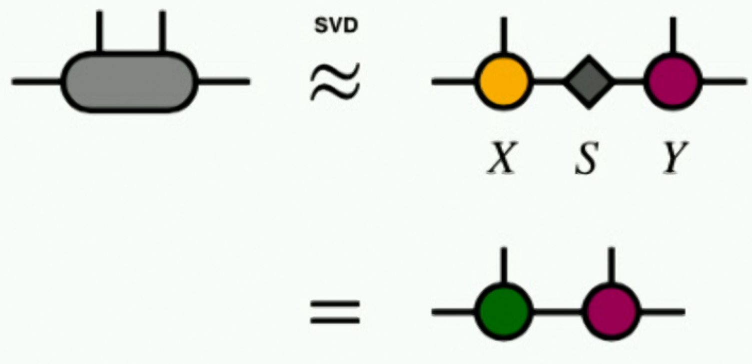


$$i = \alpha + N_\alpha \alpha' \text{ and } j = \beta + N_\beta \beta'$$

$$\hat{U}_{ij} \equiv U_{\alpha(i)\beta(j)\alpha'(i)\beta'(j)}.$$

TENSOR NETWORKS 101

<u>Compressing</u> (grouping, svd, degrouping)

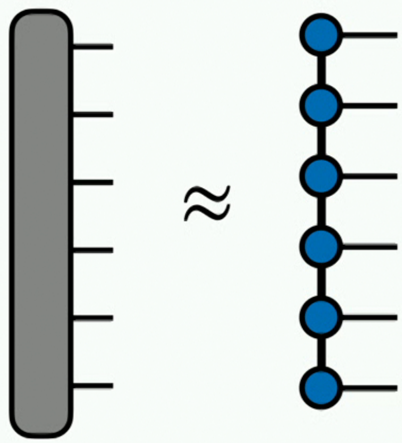


Truncated singular value decomposition provides the optimum low rank approximation of a matrix

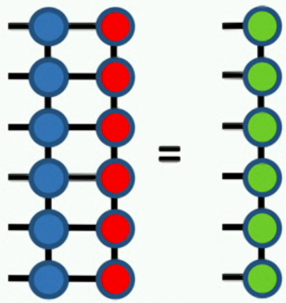
By far the most popular tensor network: Matrix Product State (MPS) or Tensor Train (TT)

$$|\Psi\rangle = \sum_{i_1 \dots i_N} \sum_{\mu_1 \dots \mu_{N-1}} M^{i_1}_{\mu_1}(1) M^{i_2}_{\mu_1 \mu_2}(2) M^{i_3}_{\mu_2 \mu_3}(3) \dots M^{i_N}_{\mu_{N-1}}(N) |i_1 i_2 i_3 \dots i_N\rangle$$

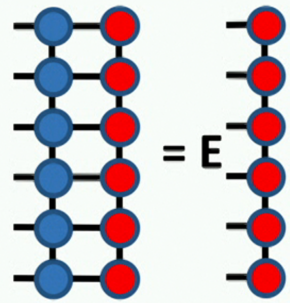
(Can be seen as a variational ansatz in e.g. DMRG)



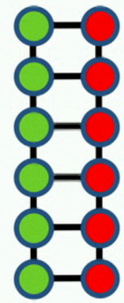
A large tool box for MPO/MPS:



A x = b



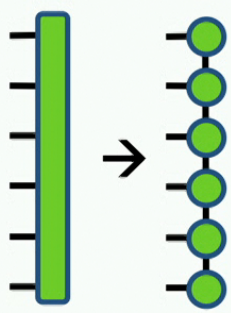
H x = E x



b^T x

(checkout ITensor from M. Stoudenmire In the room, https://itensor.org)

Tensor Cross Interpolation allows one to map many things onto this toolbox:

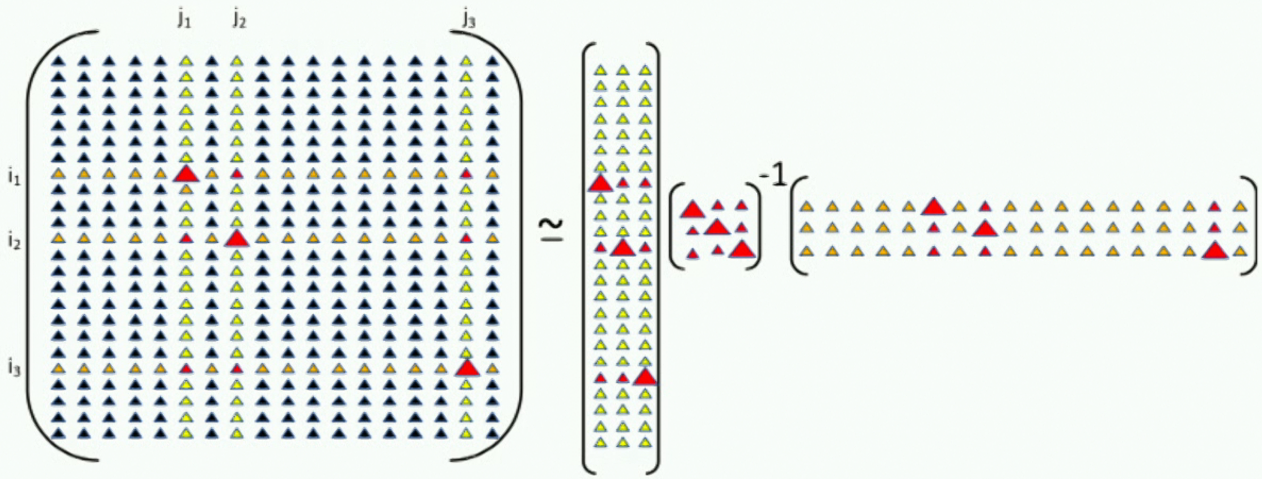


CROSS INTERPOLATION 101

- Does not necessarily require the knowledge of the full matrix.
- Approximation given as slices of the original matrices.
- In its optimum version CI is to SVD what the infinite norm is to the L_2 norm.

$$A = A \; A^{-1} \; A$$

$$A = A(\mathbb{I}, \mathbb{J}) \approx A(\mathbb{I}, \mathcal{J}) A(\mathcal{I}, \mathcal{J})^{-1} A(\mathcal{I}, \mathbb{J})$$



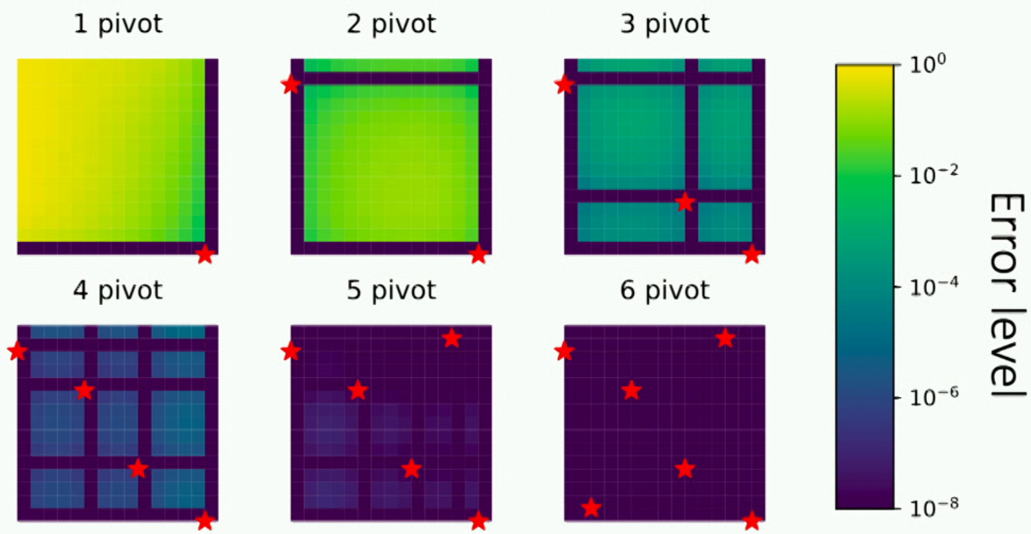
$$\mathcal{J} = \{j_1, j_2, \ldots, j_\chi\}$$
$$\mathbb{J} = \{1, 2, \ldots, N\}$$

$$A = A(\mathbb{I}, \mathbb{J}) \approx A(\mathbb{I}, \mathcal{J}) A(\mathcal{I}, \mathcal{J})^{-1} A(\mathcal{I}, \mathbb{J})$$

(P1) It is an interpolation, i.e. it is exact for any $i \in \mathcal{I}$ or $j \in \mathcal{J}$. This can be straightforwardly checked from the definition as e.g. $A(\mathcal{I}, \mathcal{J}) A(\mathcal{I}, \mathcal{J})^{-1} A(\mathcal{I}, \mathbb{J}) = A(\mathcal{I}, \mathbb{J})$.

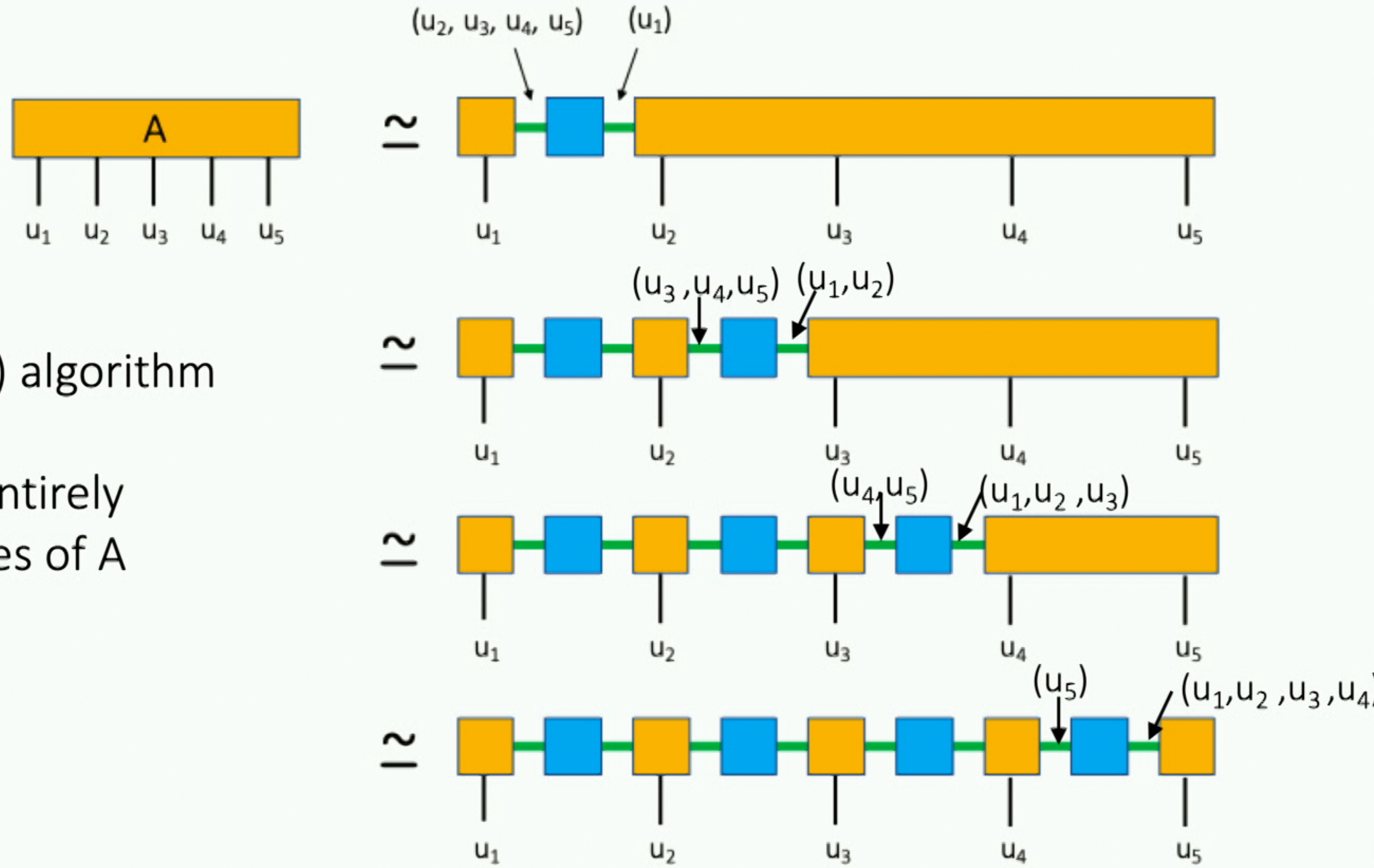
(P2) It is exact if the matrix A has rank χ (cf. Appendix B for a simple proof).

An example of Cross Interpolation



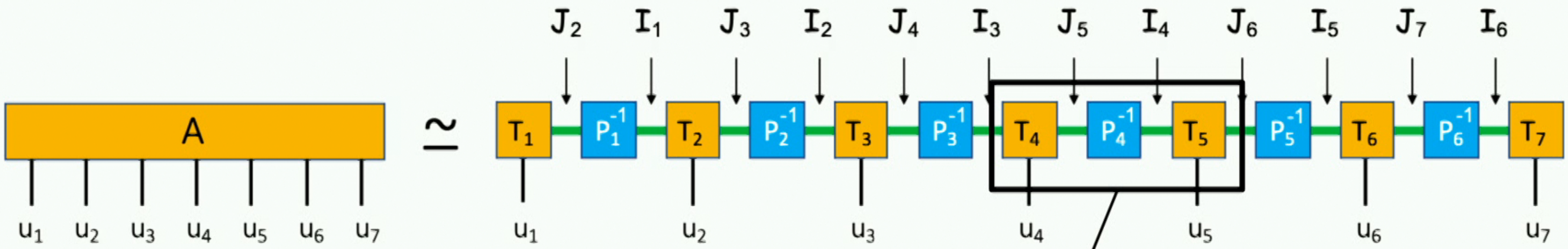
$$M(i,j) = 1 + (i/N)^2 \cos(\frac{ij}{N^2}) + (j/N)^2 \sin(\frac{ij}{N^2}) + \frac{i}{j+1}$$

TENSOR CROSS INTERPOLATION



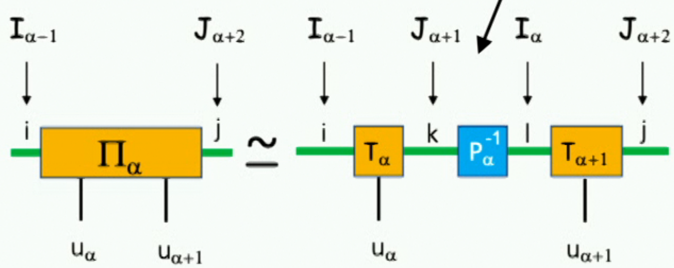
- toy (exponential) algorithm
- approximation entirely made out of slices of A

THE ACTUAL ALGORITHM (OLD VERSION)



- Initialize with a rank 1 approximation (a single call to the integrand)
- Loop over pairs of « T » to improve the cross approximation (add pivots)

$$(u_1, \ldots, u_n) = (u_1, \ldots, u_\alpha) \oplus (u_{\alpha+1}, \ldots, u_n)$$

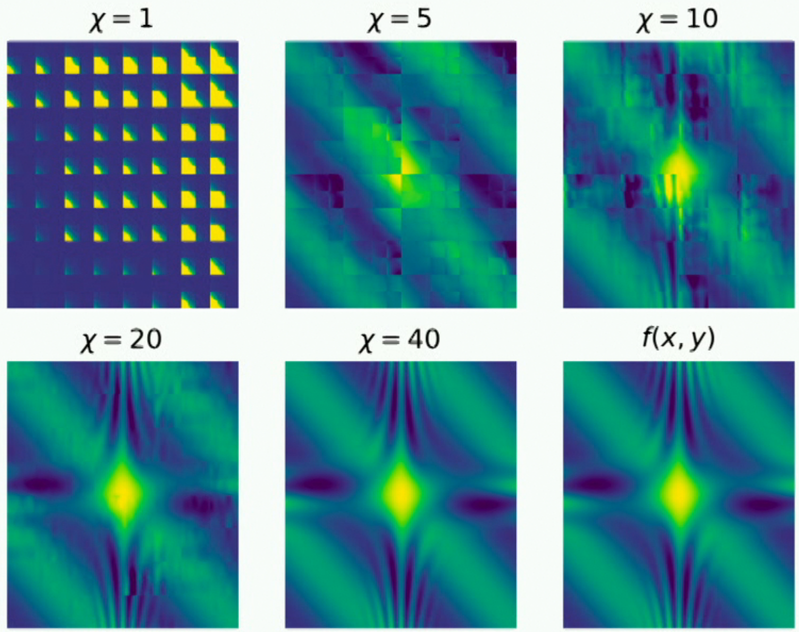


S. Dolgov and D. Savostyanov, Parallel cross interpolation for high-precision calculation of high-dimensional integrals, Computer Physics Communications **246**, 106869 (2020).

Example: « quantics » , representation of low dimension function with exponential (2^n) resolution

$$f(x,y) = e^{-0.4(x^2+y^2)} + 1 + sin(xy)e^{-x^2} + cos(3xy)e^{-y^2} + cos(x+y)$$

$$x = \frac{x_1}{2} + \frac{x_2}{2^2} + \frac{x_3}{2^3} + \ldots + \frac{x_n}{2^n} \qquad x_i \in \{0,1\}$$



Today:

1) Tensor Trains & the Tensor Cross interpolation algorithm.
2) Application to the calculation of Feynman diagrams.
3) Some Kondo physics.

TOOLS FOR QUANTUM TRANSPORT

$$\hat{H} = \sum_{ij} H_{ij} c_i^\dagger c_j$$

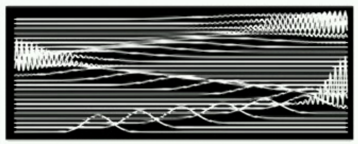
kwant

HTTP://KWANT-PROJECT.ORG

With TU Delft (Akhmerov, Wimmer).

Main developer: C. Groth

$$\hat{H}(t) = \sum_{ij} H_{ij}(t) c_i^+ c_j$$



HTTP://TKWANT.KWANT-PROJECT.ORG

Main developer: T. Kloss

$$\hat{\mathbf{H}}(t) = \hat{\mathbf{H}}_0(t) + U\hat{\mathbf{H}}_{\text{int}}(t)$$

$$\hat{\mathbf{H}}_{\text{int}}(t) = \sum_{ijkl} \mathbf{V}_{ijkl}(t) \hat{\mathbf{c}}_i^\dagger \hat{\mathbf{c}}_j^\dagger \hat{\mathbf{c}}_k \hat{\mathbf{c}}_l.$$

?

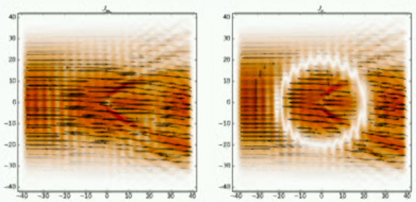
- Kondo physics
- Coulomb blockade, Fermi edge singularity
- 0.7 anomaly
- FQHE
- Quantum computers

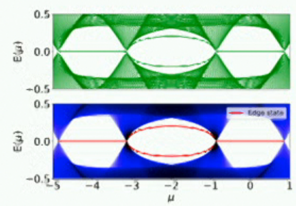
...

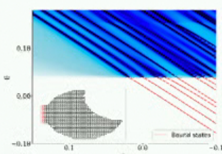
KWANT GALLERY

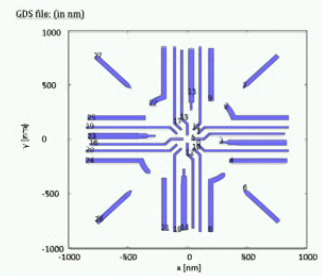
HTTP://KWANT-PROJECT.ORG

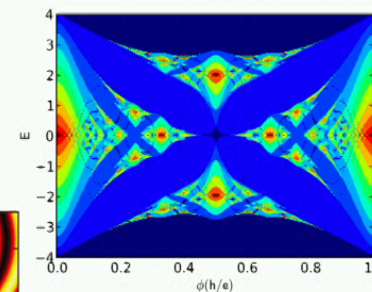
With TU Delft (Akhmerov, Wimmer et al.)

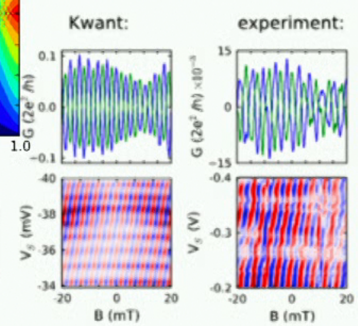


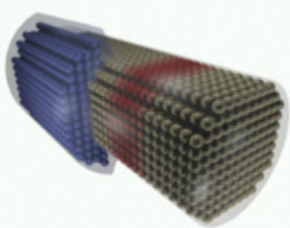


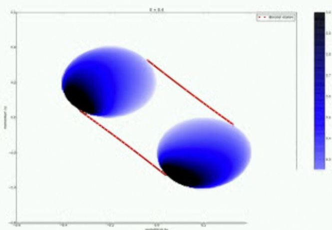


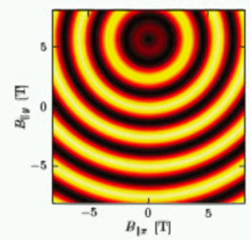


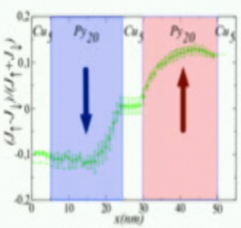


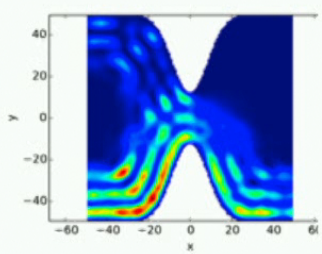


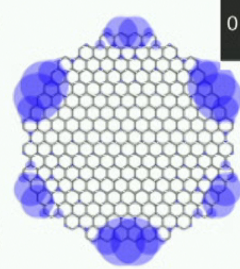


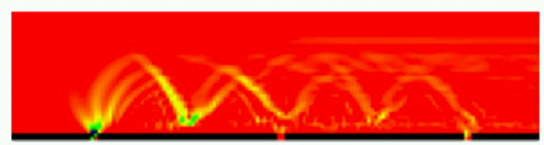






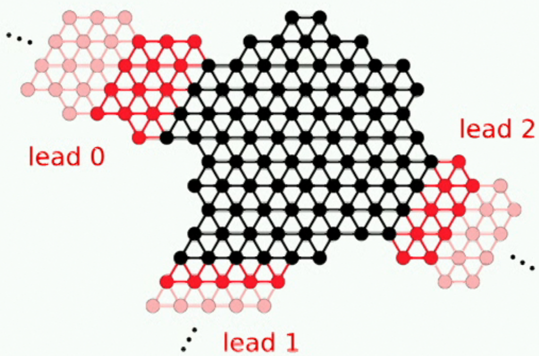




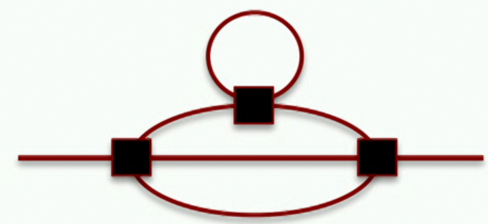


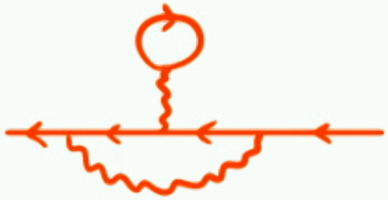
$$\hat{\mathbf{H}}(t) = \hat{\mathbf{H}}_0(t) + U\hat{\mathbf{H}}_{\text{int}}(t)$$

$$\hat{\mathbf{H}}_{\text{int}}(t) = \sum_{ijkl} \mathbf{V}_{ijkl}(t)\hat{\mathbf{c}}_i^\dagger \hat{\mathbf{c}}_j^\dagger \hat{\mathbf{c}}_k \hat{\mathbf{c}}_l.$$



$$Q(U) = \sum_{n=0}^{+\infty} Q_n U^n$$



A VERY BRAVE/STUPID APPROACH: 

→ CALCULATE ALL THE FEYNMAN DIAGRAMS UP TO A GIVEN (LARGE) ORDER

$$F(U) = \sum_n F_n U^n$$

- PROBLEM #1: There are n! diagrams.
- PROBLEM #2 How to calculate n dimensional integrals
- PROBLEM #3 How to reconstruct F(U) from the F_n .

$$q_n(t=\infty) \sim \frac{1}{r^n} \qquad q_n(t) \sim \frac{1}{n!}\, t^n$$

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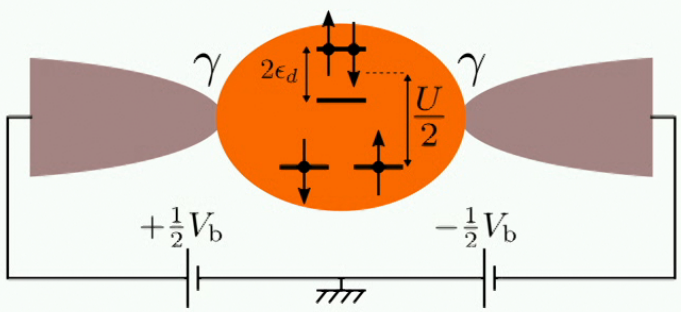
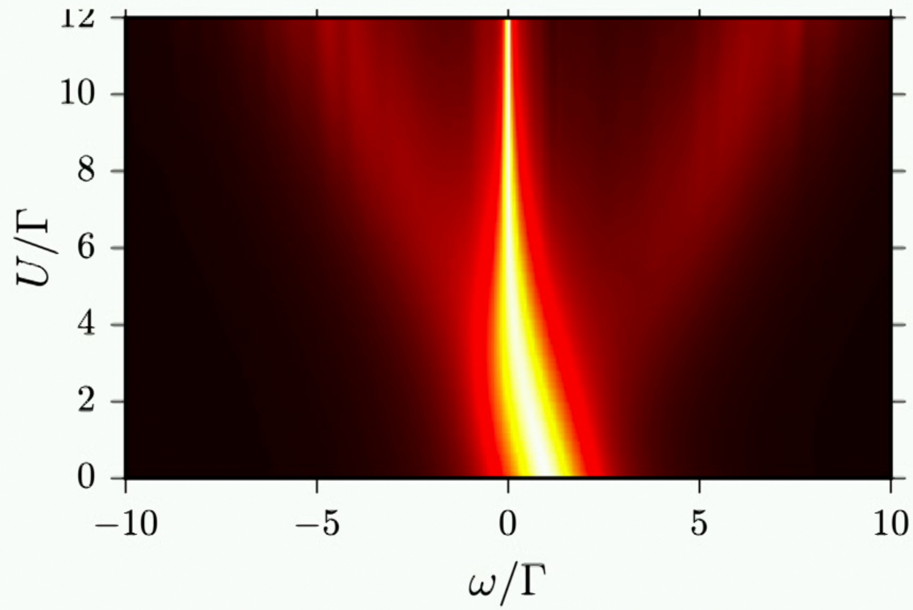
TEASER: AT EQUILIBRIUM





$$\hat{\mathbf{H}} = \sum_{i=-\infty}^{+\infty} \sum_{\sigma} \gamma_i \hat{\mathbf{c}}_{i,\sigma}^{\dagger} \hat{\mathbf{c}}_{i+1,\sigma} + h.c. + \epsilon_d(\hat{\mathbf{n}}_{\uparrow} + \hat{\mathbf{n}}_{\downarrow}) + U\theta(t)\left(\hat{\mathbf{n}}_{\uparrow} - \frac{1}{2}\right)\left(\hat{\mathbf{n}}_{\downarrow} - \frac{1}{2}\right).$$

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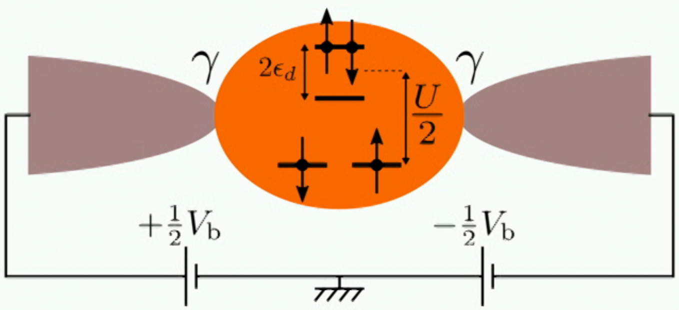
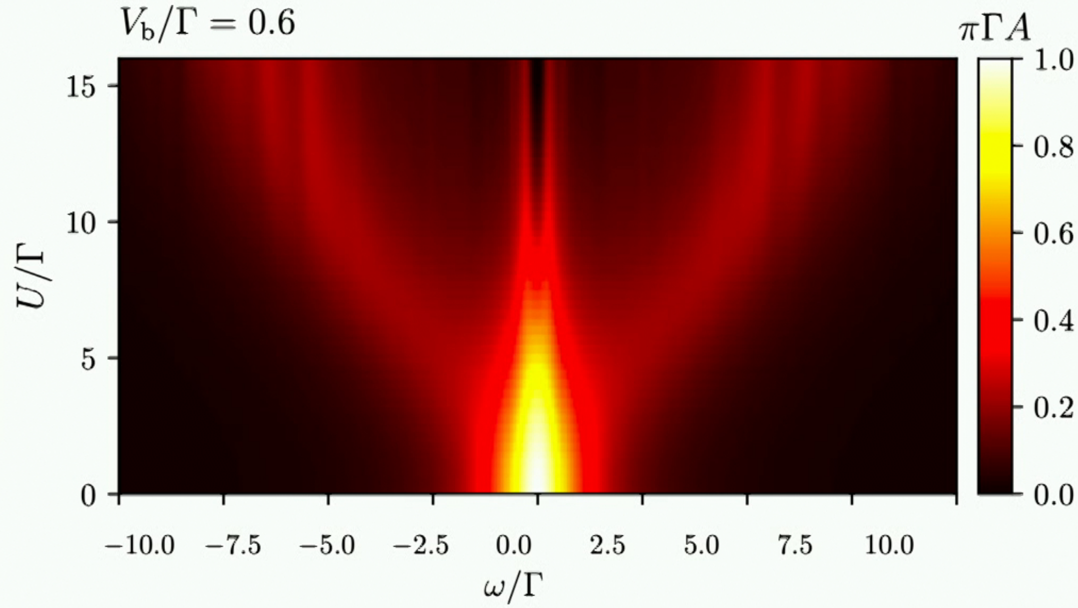
TEASER: OUT-OF-EQUILIBRIUM





$$\hat{\mathbf{H}} = \sum_{i=-\infty}^{+\infty} \sum_{\sigma} \gamma_i \hat{\mathbf{c}}^{\dagger}_{i,\sigma} \hat{\mathbf{c}}_{i+1,\sigma} + h.c. + \epsilon_d(\hat{\mathbf{n}}_{\uparrow} + \hat{\mathbf{n}}_{\downarrow}) + U\theta(t) \left(\hat{\mathbf{n}}_{\uparrow} - \frac{1}{2}\right) \left(\hat{\mathbf{n}}_{\downarrow} - \frac{1}{2}\right).$$

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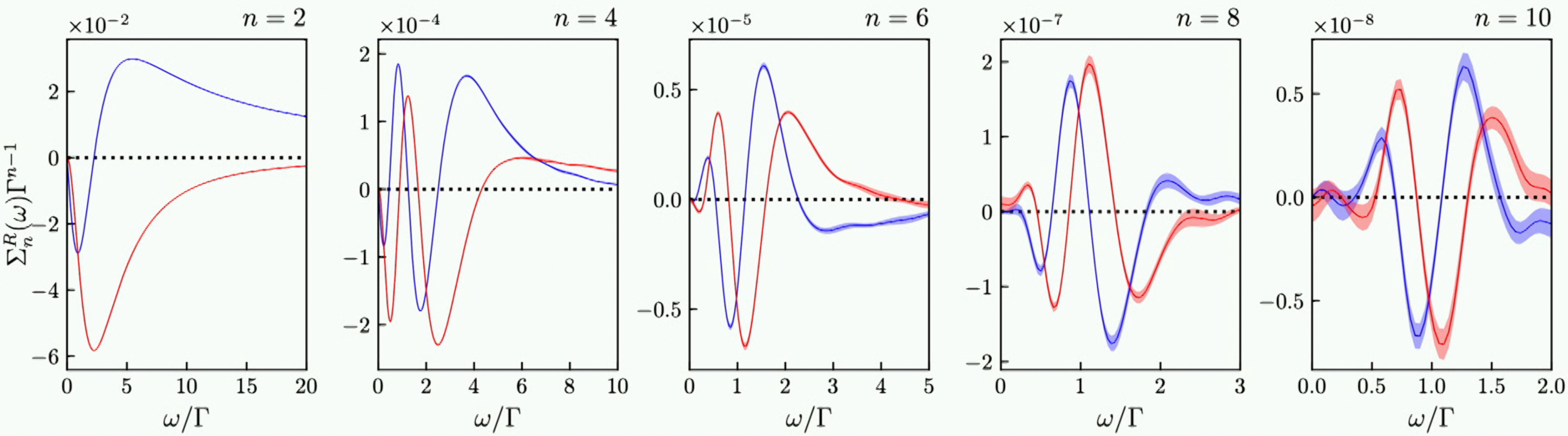
PROBLEM #1: THE N! DIAGRAMS

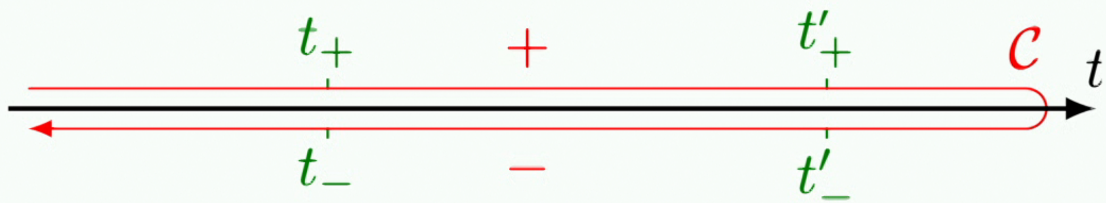


(« old » data, using diagrammatic Monte-Carlo)

KELDYSH FORMALISM IN A NUTSHELL

$$\langle \mathcal{O}(t) \rangle = \langle \mathcal{U}^\dagger(t) \mathcal{O} \mathcal{U}(t) \rangle$$

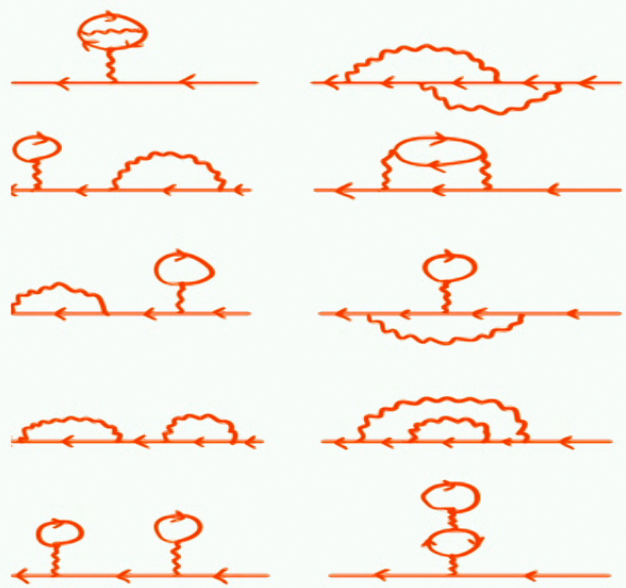
$$\mathcal{U}(t) = T \exp\left(-i \int_0^t \hat{H}_{\rm int}(u) du \right)$$



$$\langle \mathcal{O}(t) \rangle = \left\langle T_{\mathcal{C}} \hat{\mathcal{O}}(t) \exp\left(-i \int_{\mathcal{C}} \hat{H}_{\rm int}(u) du \right) \right\rangle$$

WICK DETERMINANTS

$$\left\langle c_1^+ c_1 c_2^+ c_2 c_3^+ c_3 c_4^+ c_4 c_5^+ c_5 \right\rangle = \sum_P (-1)^{|P|} \left\langle c_1^+ c_{P(1)} \right\rangle \left\langle c_2^+ c_{P(2)} \right\rangle \left\langle c_3^+ c_{P(3)} \right\rangle \left\langle c_4^+ c_{P(4)} \right\rangle \left\langle c_5^+ c_{P(5)} \right\rangle$$



WICK DETERMINANTS

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$$\left\langle c_1^+ c_1 c_2^+ c_2 c_3^+ c_3 c_4^+ c_4 c_5^+ c_5 \right\rangle = \det \left\langle c_i^+ c_j \right\rangle$$

A « VERY SIMPLE » FORMULA

$$G^c_{ij}(\bar{t},\bar{t}') = \sum_{n=0}^{+\infty} \frac{i^n}{n!} U^n \sum_{\{a_i\}} (-1)^{\sum_i a_i} \int du_1 du_2 \dots du_n \sum_{i_1 j_1 k_1 l_1} V_{i_1 j_1 k_1 l_1}(u_1) \cdots \sum_{i_n j_n k_n l_n} V_{i_n j_n k_n l_n}(u_n) \det \mathbf{M}_n$$

2ⁿ sum cancels disconnected diagrams

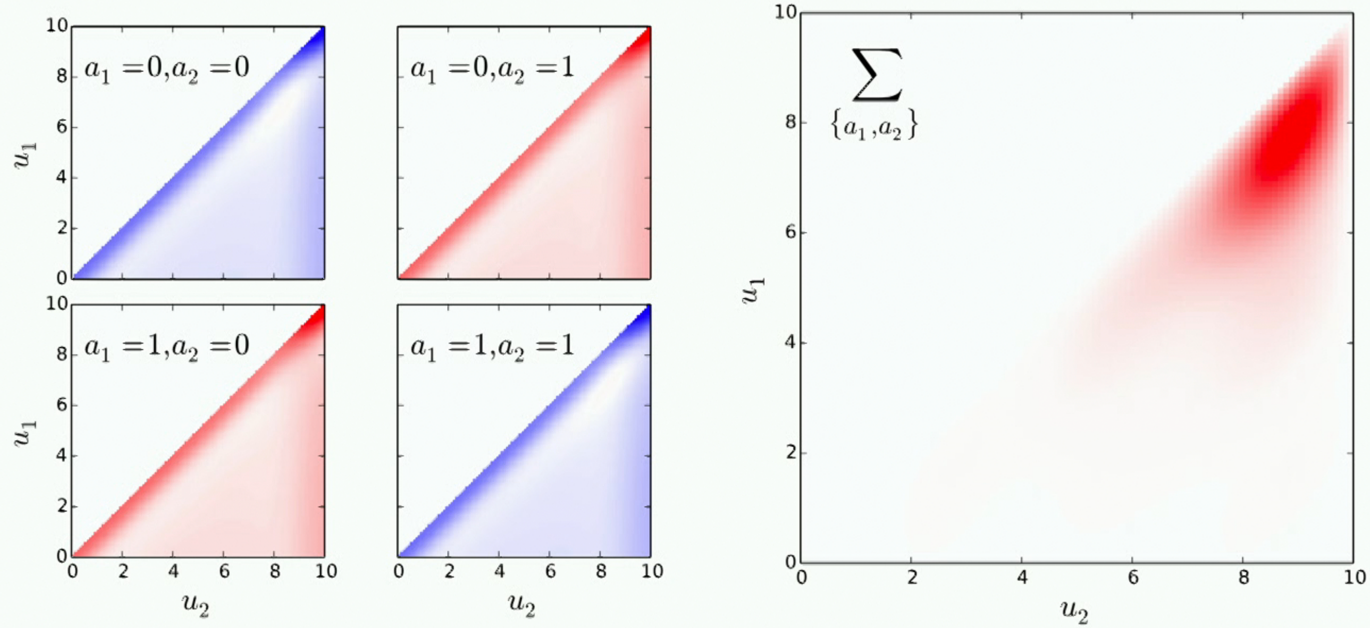
$$\mathbf{M}_n = \begin{pmatrix} g^<_{k_1 i_1}(\bar{u}_1,\bar{u}_1) & g^<_{k_1 j_1}(\bar{u}_1,\bar{u}_1) & g^c_{k_1 i_2}(\bar{u}_1,\bar{u}_2) & \dots & g^c_{k_1 j}(\bar{u}_1,\bar{t}') \\ g^<_{l_1 i_1}(\bar{u}_1,\bar{u}_1) & g^<_{l_1 j_1}(\bar{u}_1,\bar{u}_1) & g^c_{l_1 i_2}(\bar{u}_1,\bar{u}_2) & \dots & g^c_{l_1 j}(\bar{u}_1,\bar{t}') \\ g^c_{k_2 i_1}(\bar{u}_2,\bar{u}_1) & g^c_{k_2 j_1}(\bar{u}_2,\bar{u}_1) & g^<_{k_2 i_2}(\bar{u}_2,\bar{u}_2) & \dots & g^c_{k_2 j}(\bar{u}_2,\bar{t}') \\ \dots & \dots & \dots & \dots & \dots \\ g^c_{k_n i_1}(\bar{u}_n,\bar{u}_1) & g^c_{k_n j_1}(\bar{u}_n,\bar{u}_1) & g^c_{k_n i_2}(\bar{u}_n,\bar{u}_2) & \dots & g^c_{k_n j}(\bar{u}_n,\bar{t}') \\ g^c_{l_n i_1}(\bar{u}_n,\bar{u}_1) & g^c_{l_n j_1}(\bar{u}_n,\bar{u}_1) & g^c_{l_n i_2}(\bar{u}_n,\bar{u}_2) & \dots & g^c_{l_n j}(\bar{u}_n,\bar{t}') \\ g^c_{i i_1}(\bar{t},\bar{u}_1) & g^c_{i j_1}(\bar{t},\bar{u}_1) & g^c_{i i_2}(\bar{t},\bar{u}_2) & \dots & g^c_{ij}(\bar{t},\bar{t}') \end{pmatrix}$$

$$g^<_{ij}(t,t') = i \sum_\alpha \int \frac{dE}{2\pi} f_\alpha(E) \Psi_{\alpha E}(t,i) \Psi^*_{\alpha E}(t',j) + i \sum_n f(E_n) \Psi_n(t,i) \Psi^*_n(t',j)$$

Known non-interacting functions.

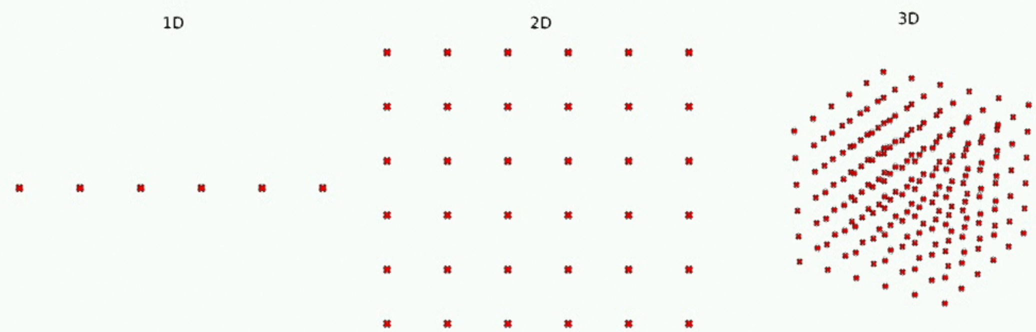
$$G^c_{ij}(\bar{t},\bar{t}') = \sum_{n=0}^{+\infty} \frac{i^n}{n!} U^n \sum_{\{a_i\}} (-1)^{\sum_i a_i} \int du_1 du_2 \ldots du_n \sum_{i_1 j_1 k_1 l_1} V_{i_1 j_1 k_1 l_1}(u_1) \cdots \sum_{i_n j_n k_n l_n} V_{i_n j_n k_n l_n}(u_n) \det \mathbf{M}_n$$

2^n sum cancels disconnected diagrams



PROBLEM #2 THE N DIMENSIONAL INTEGRAL

→ The dimensionality curse,
L^d points.



$$Q(U) = \sum_n Q_n U^n$$

$$Q_n = \int dv_1 \ldots dv_n \; \tilde{Q}_n(v_1, \ldots, , v_n).$$

The standard approach: Metropolis Monte-Carlo.
→ Intrinsic very slow convergence $N^{-1/2}$ (as opposed to $1/N^{15}$ or even exponential in 1D)
→ We do not build any knowledge of f(u)
→ The infamous sign problem.

MACHINE LEARNING THE INTEGRAND

What if the integrand factorized?

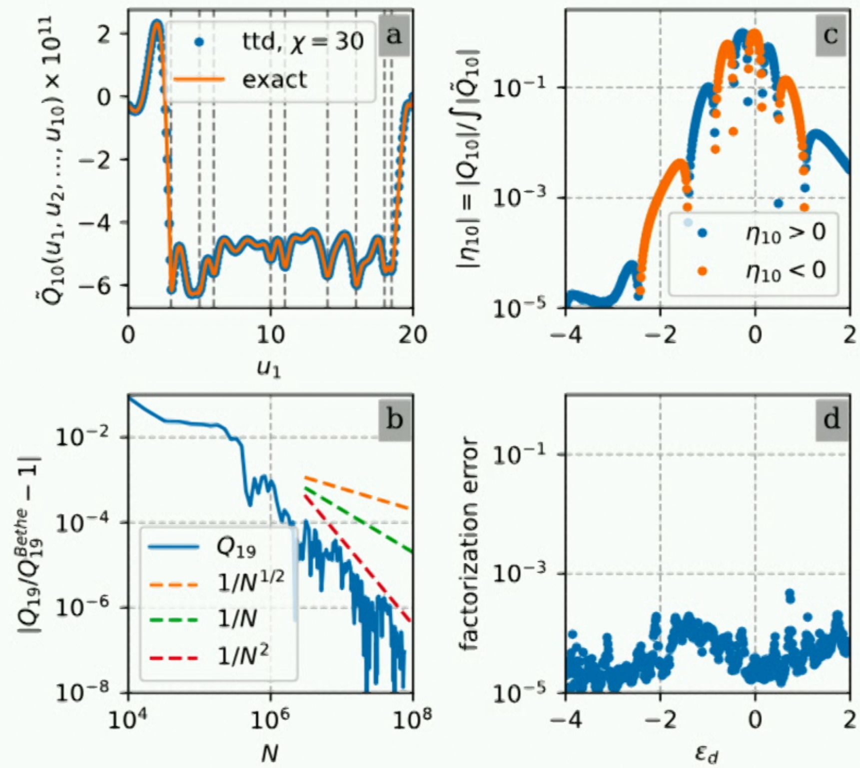
$$\tilde{Q}_n(v_1, \ldots, v_n) \approx M_1(v_1) \cdots M_n(v_n)$$

Then the integration would be trivial

$$Q_n \approx \left(\int dv_1 M_1(v_1) \right) \cdots \left(\int dv_n M_n(v_n) \right)$$

→ A job for Tensor Cross Interpolation

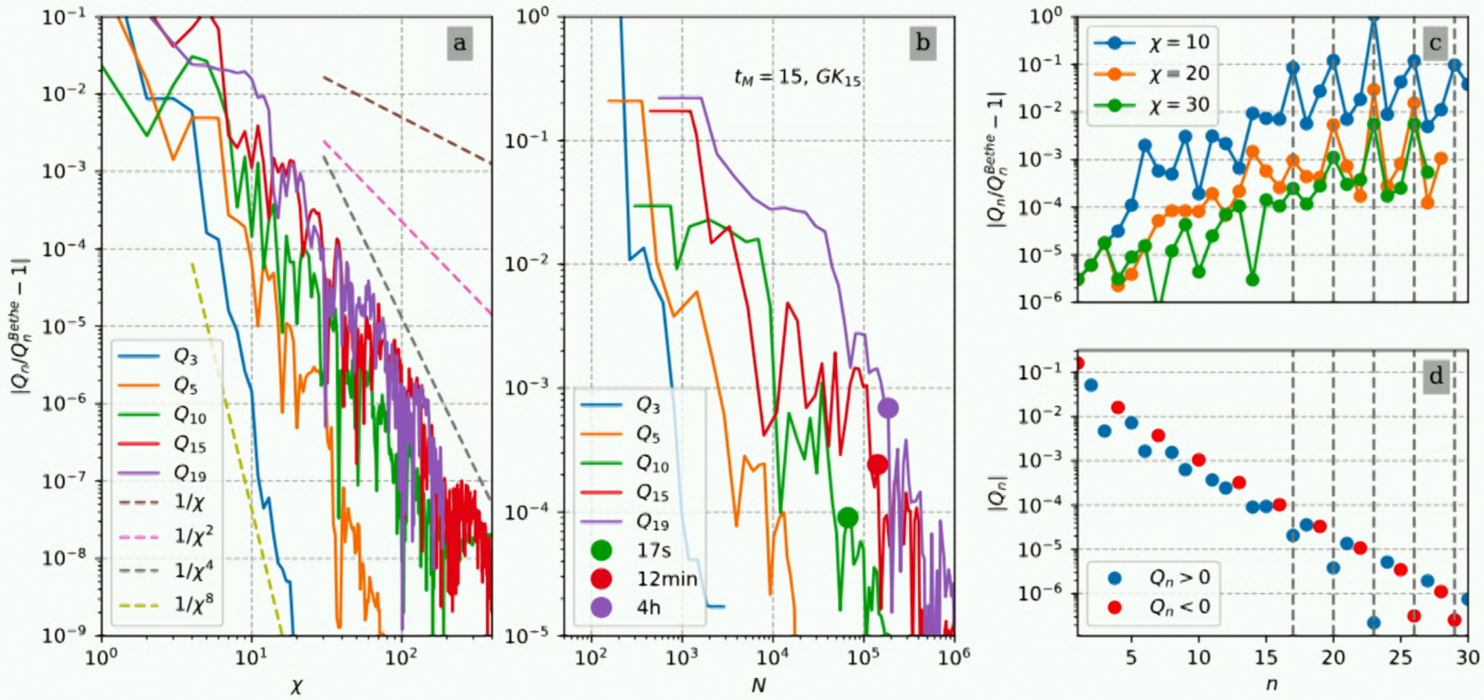
BENCHMARKING THE RESULTS



Unprecedented convergence

Agnostic to sign problem

BENCHMARKING THE RESULTS



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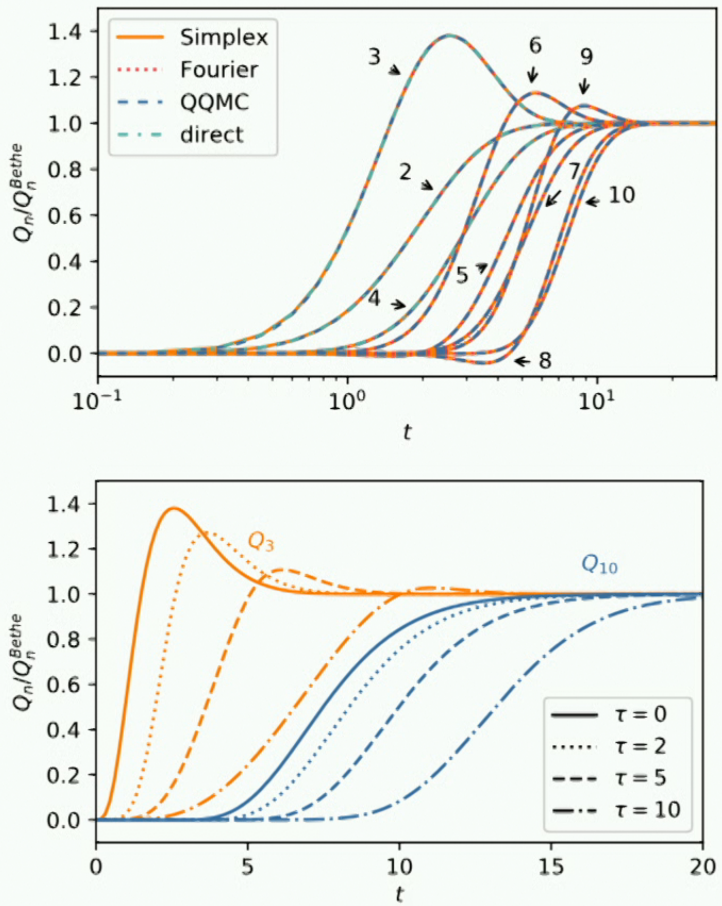
INTEGRATION IS A COSTLESS POST PROCESSING STEP



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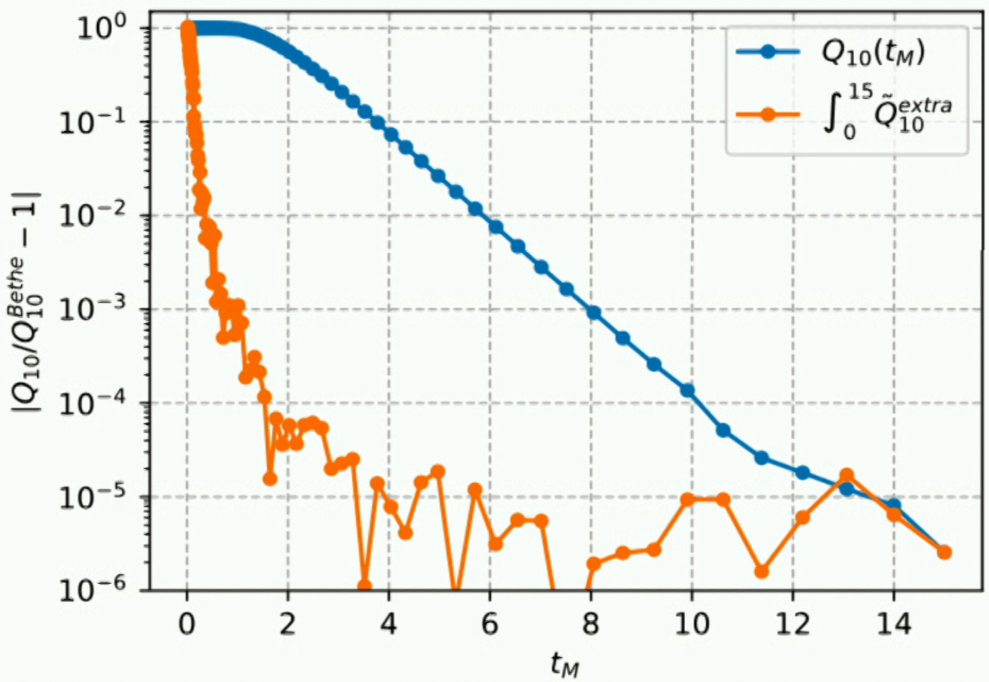
THIS IS MORE THAN INTERPOLATION



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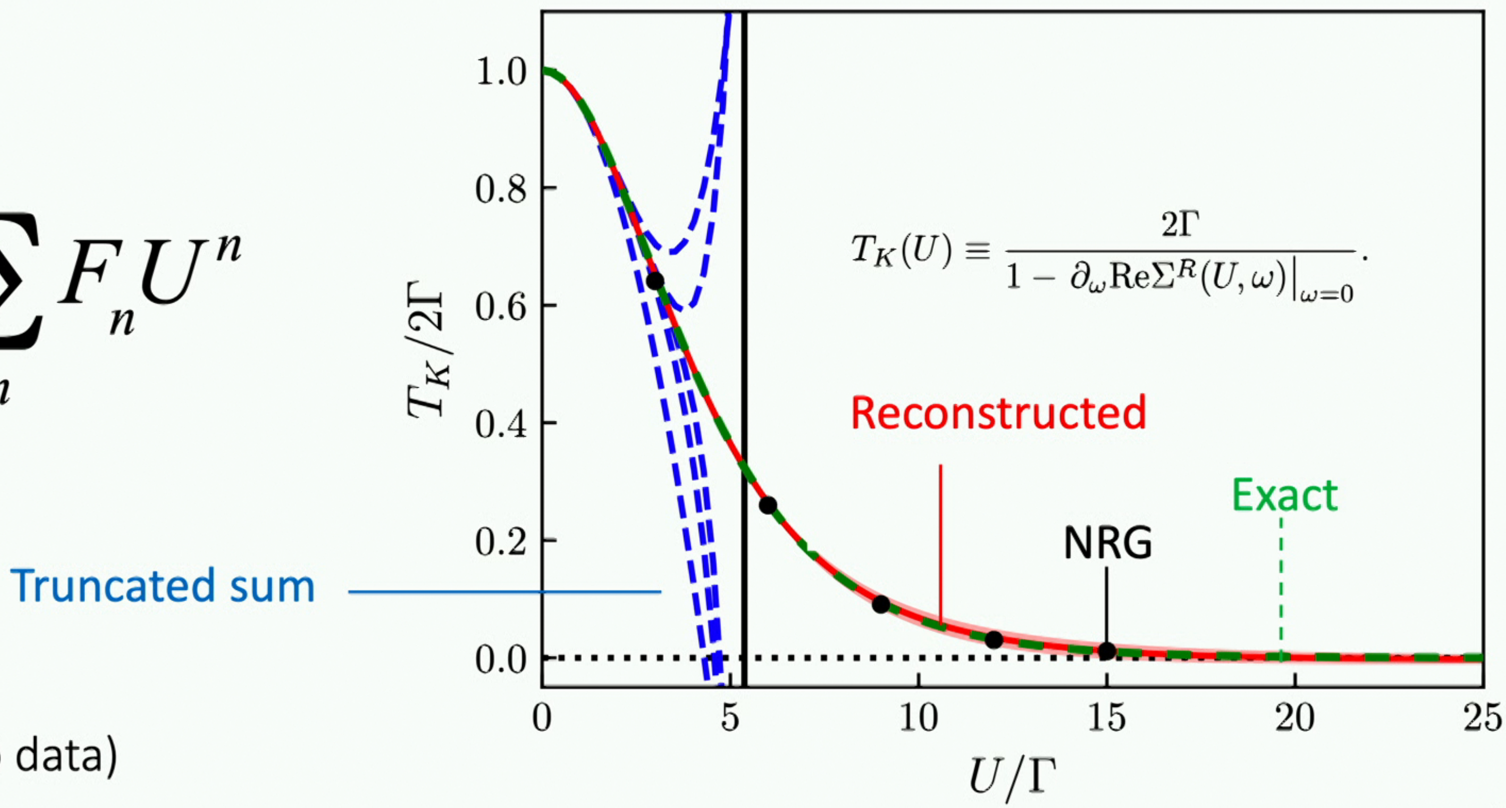
PROBLEM #3: RECONSTRUCTRING F(U) FROM F_N

$$F(U) = \sum_n F_n U^n$$

(Monte-Carlo data)



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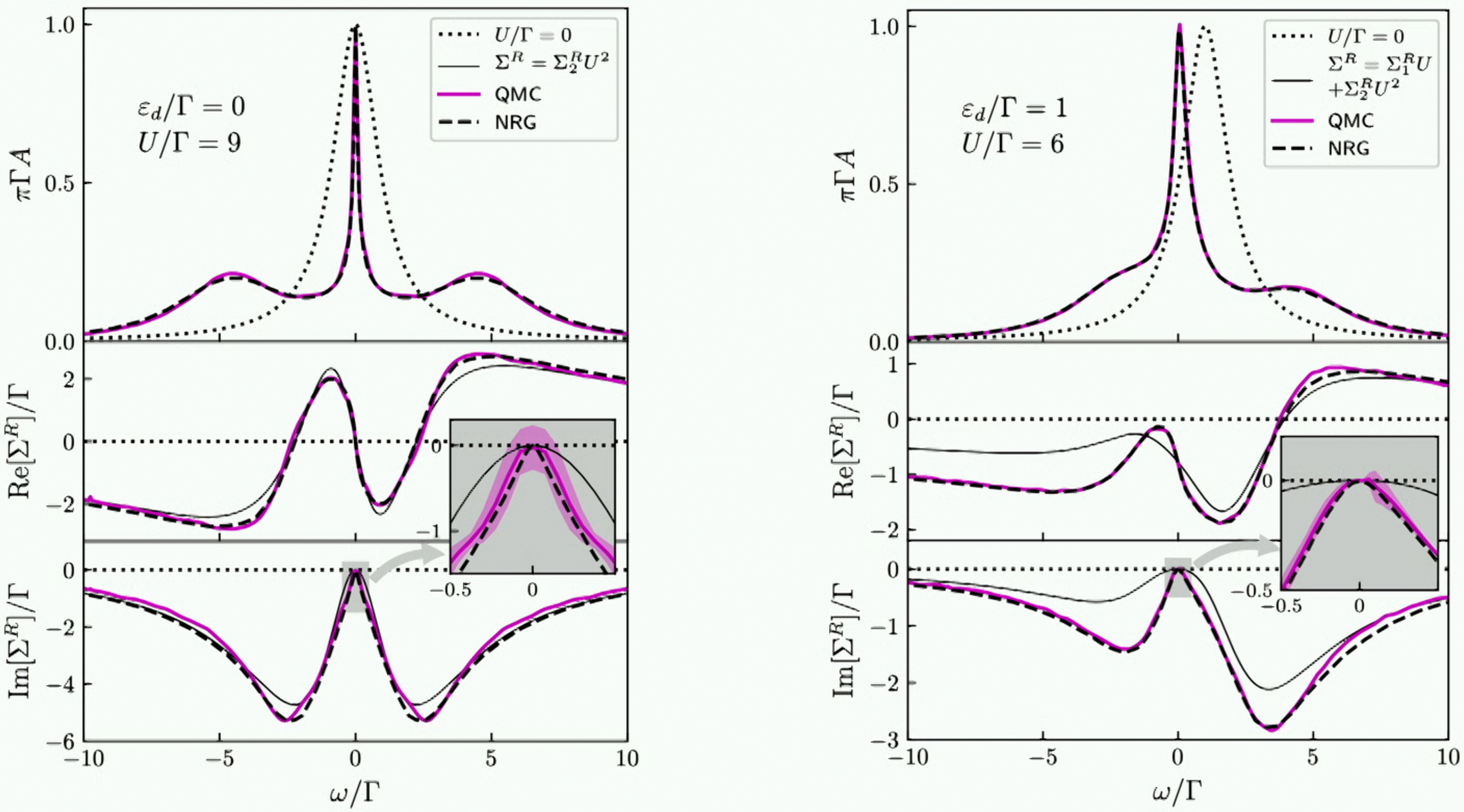
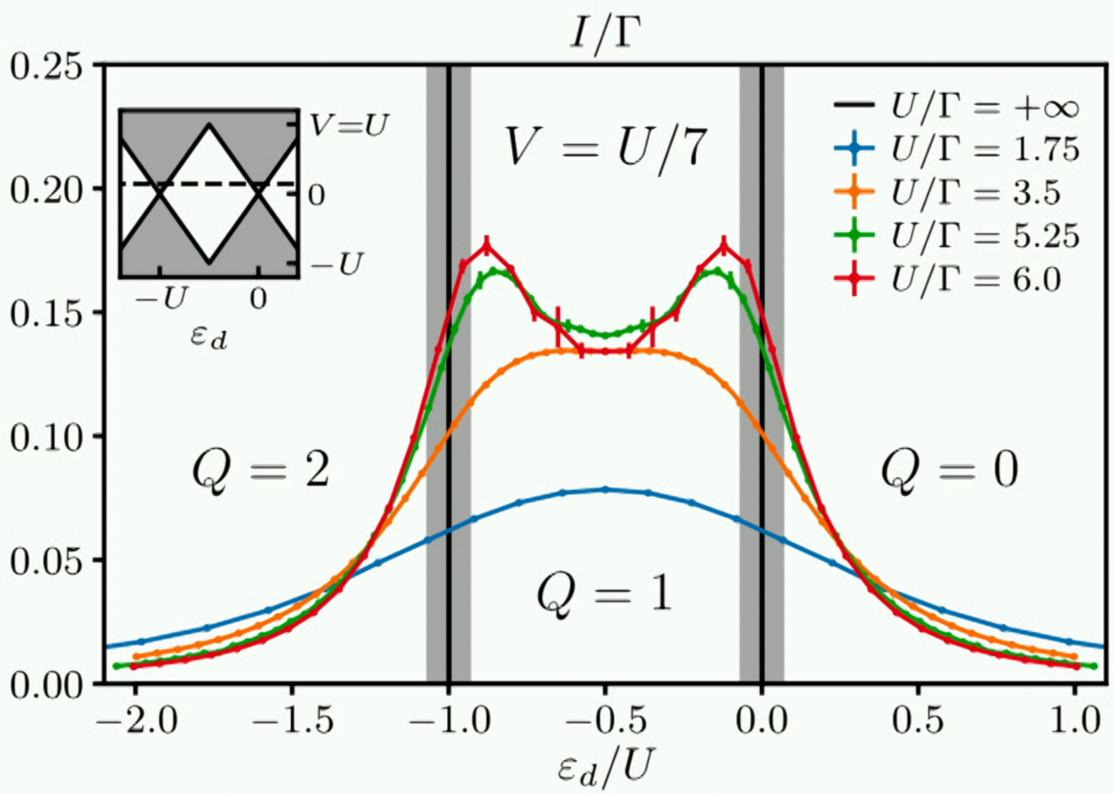
SOME EQUILIBRIUM BENCHMARKS



(Monte-Carlo data)

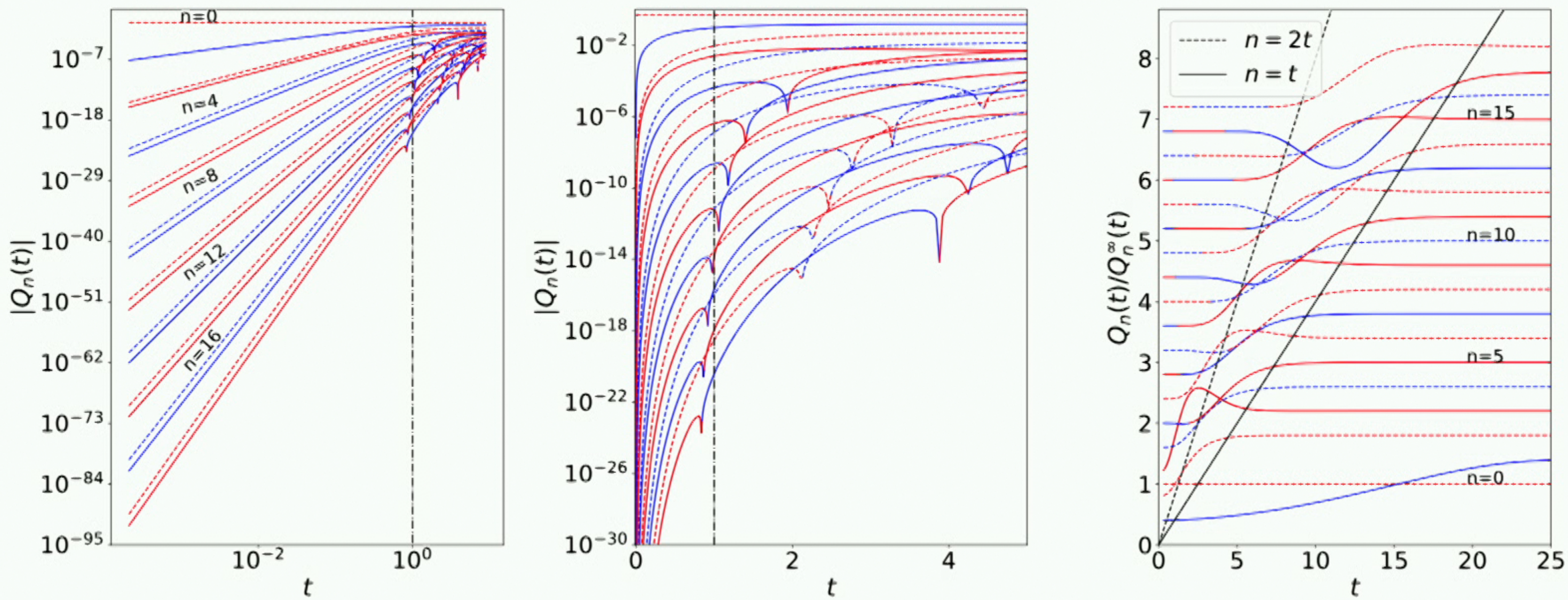
AND BACK TO NON-EQUILIBRIUM



(low discrepancy
sequence integratic
data

40

Data with the new tensor train technique



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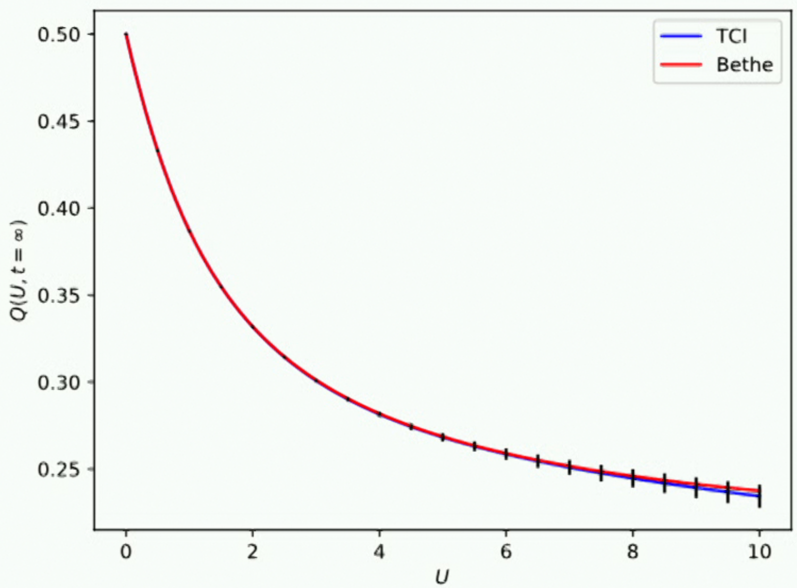
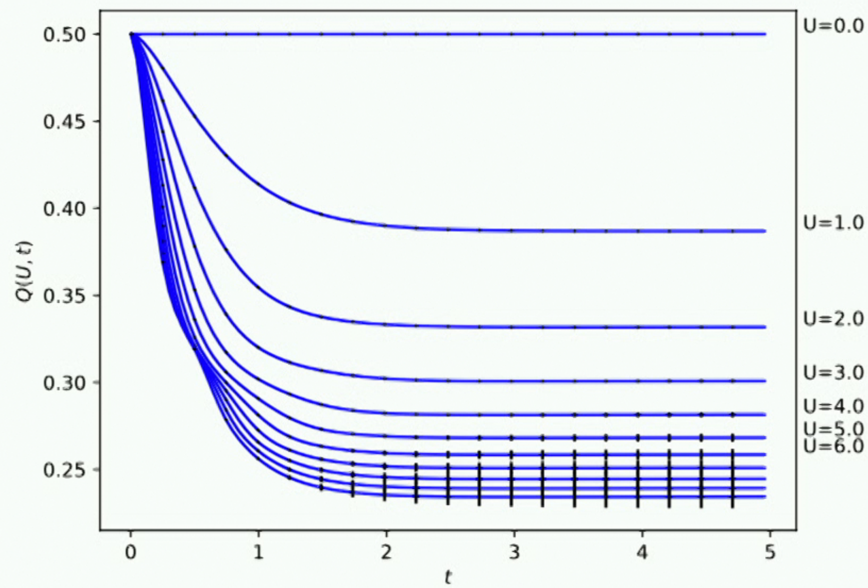
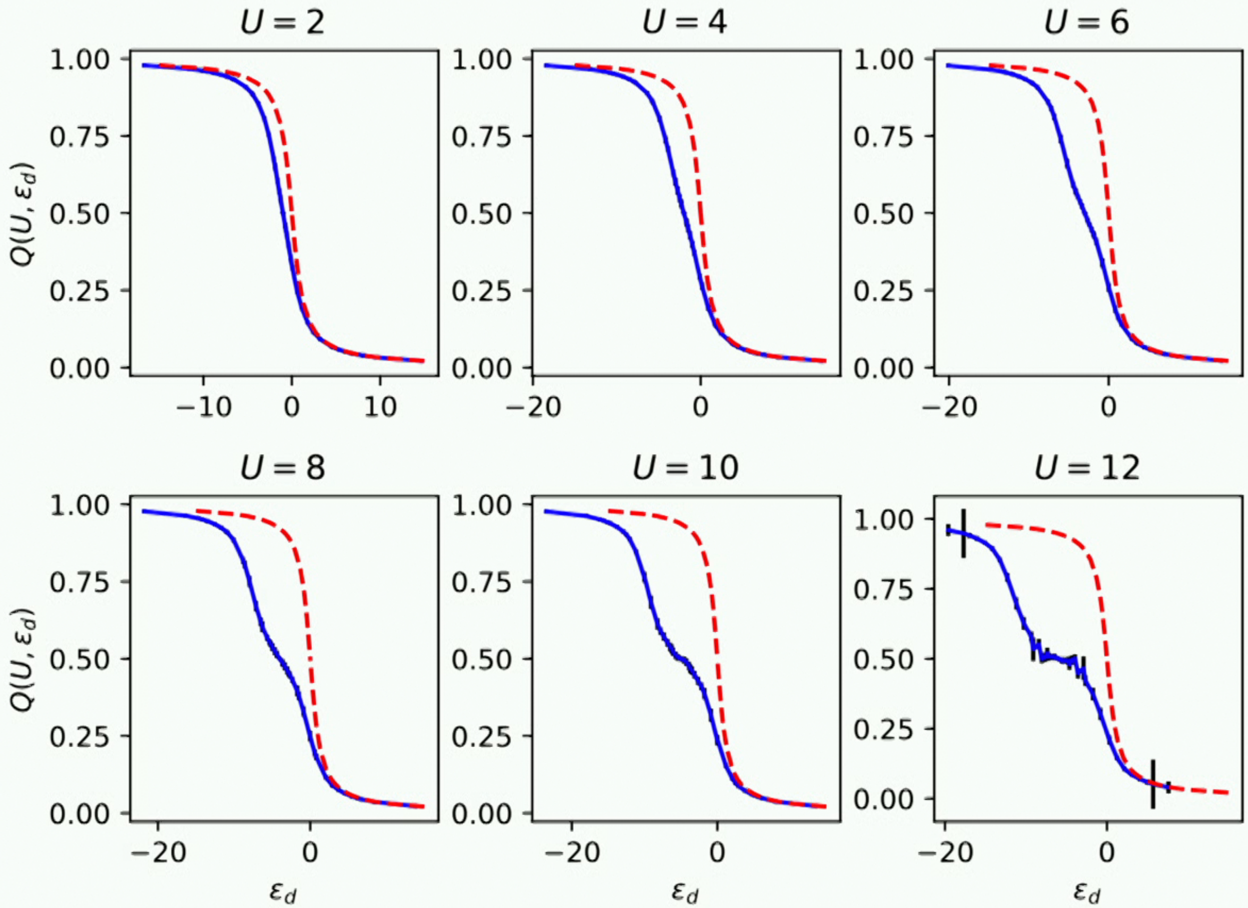
Data with the new tensor train technique



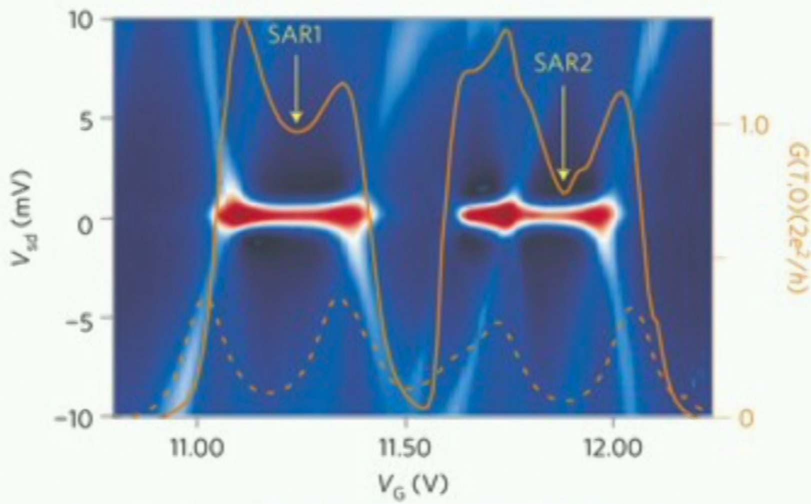


$$Q(U,t) \approx \sum_{n=0}^{N} q_n(t) U^n$$

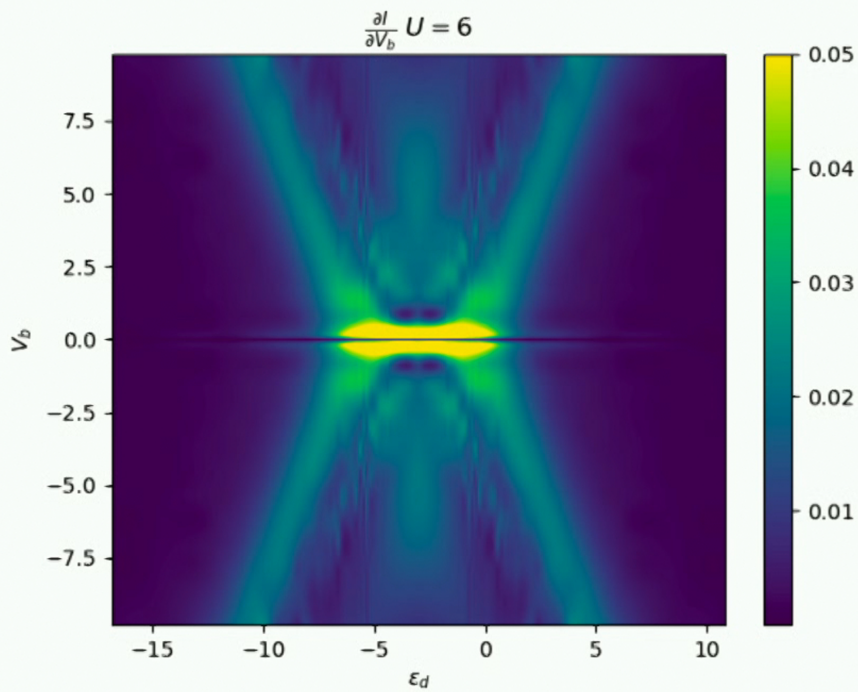
Data with the new tensor train technique



Data with the new tensor train technique



Nature Physics **5**, 208 (2009)



Caution: fresh from the oven)

CONCLUSION

- In principle, tensor cross-interpolation can be used (tried) wherever Monte-Carlo has been.

→ that's a lot of things to explore (imaginary time, quantum field approaches, classical problems…) → Got started on hybridization expansion **arXiv:2303.11199**

- It can also be used for other problems (quantics/superfast FFT, learning an experiment, ising models) **arXiv:2303.11819**
- We do not know yet how far we will be able to go with our tensor train diagrammatic approach

→ Hubbard models, DMFT, 0.7 anomaly, few qubits and their baths

- Open source sofware « xfac » coming up (with a better TCI algorithm).
- PEPS…

PHYSICAL REVIEW LETTERS **125**, 047702 (2020)
PHYSICAL REVIEW X **9**, 041008 (2019)
PHYSICAL REVIEW B **100**, 125129 (2019)
PHYSICAL REVIEW B **91**, 245154 (2015)

https://arxiv.org/abs/2207.06135
Phys. Rev. X 12, 041018 (2022).

I am hiring! (postdocs/PhD)

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