Memory-efficient nonequilibrium Green's function framework built on quantics tensor trains

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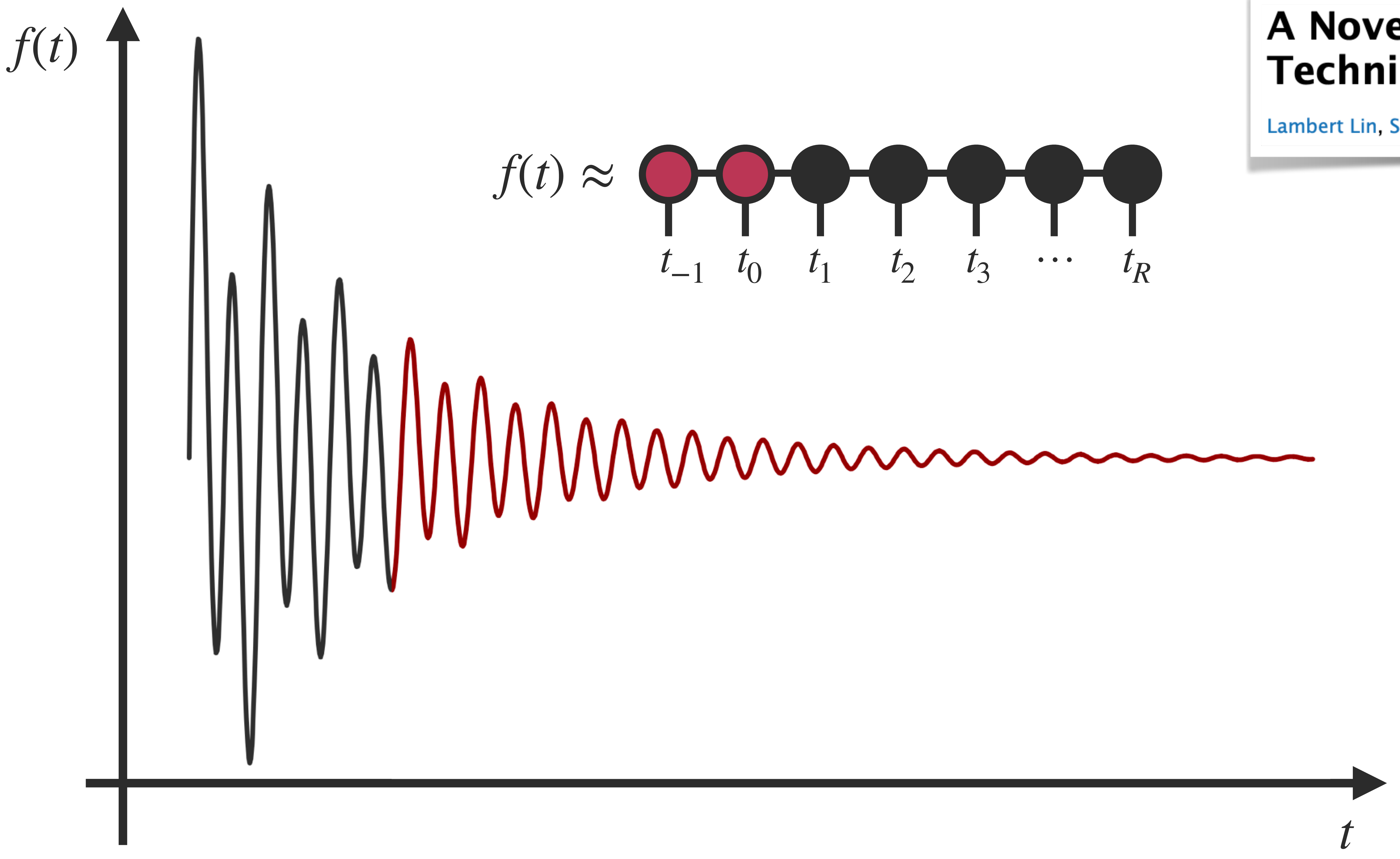


A Novel Method of Function Extrapolation Inspired by Techniques in Low-entangled Many-body Physics

Lambert Lin, Steven R White

...?

dynamic mode decomposition

Schmid, J. Fluid Mech. 656, 5–28 (2010)

$$\frac{d\mathbf{x}(t)}{dt} = \underbrace{\mathbf{f}(\mathbf{x}(t), t)}_{\text{nonlinear}} \approx \underbrace{\mathbf{A}\mathbf{x}(t)}_{\text{linear}}$$

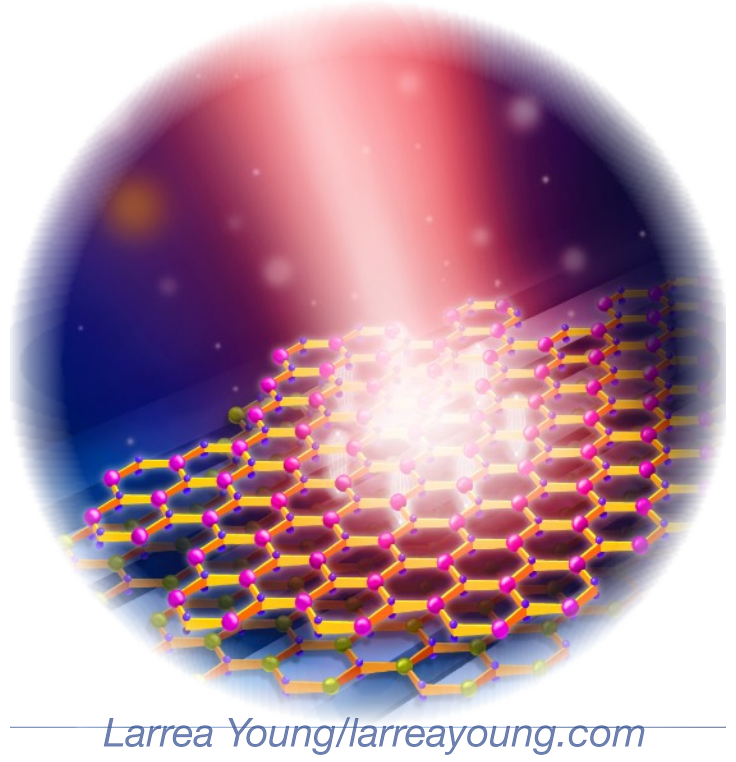
low-rank

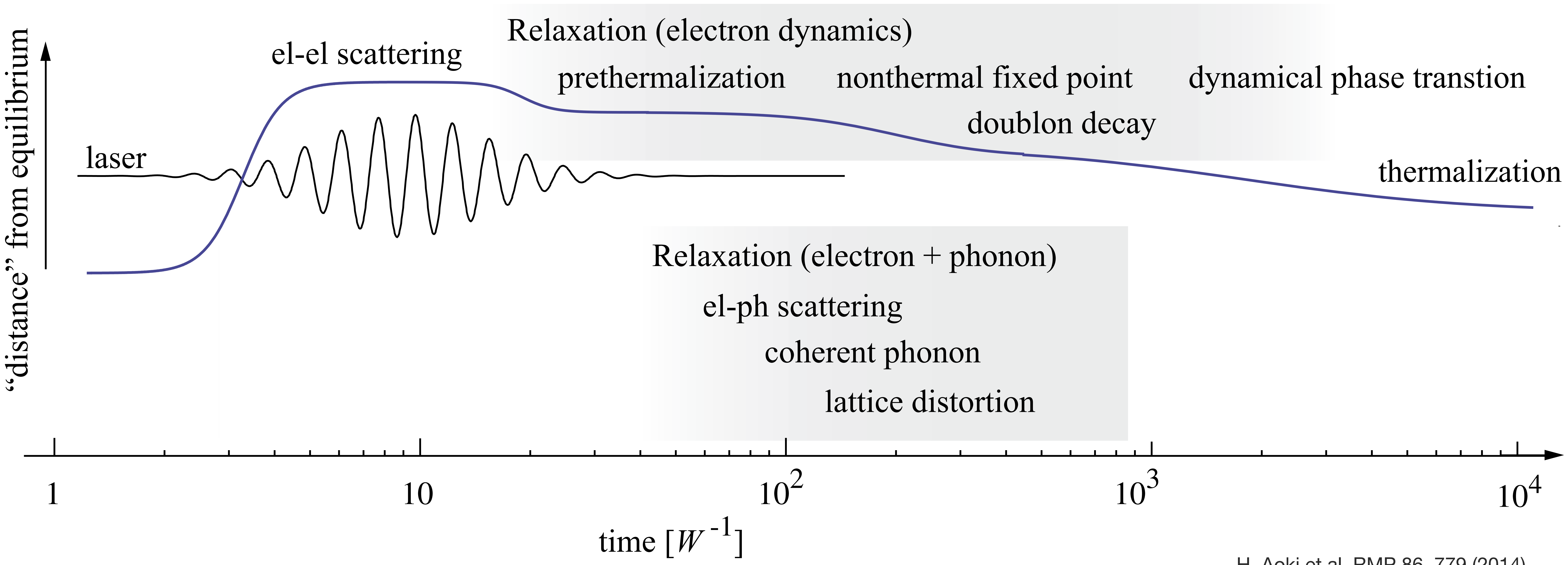
$$\mathbf{x}(t) \approx \sum_{\ell} \phi_\ell \exp\left(i\omega_\ell t\right) b_\ell$$

eigenvectors and eigenvalues of $\mathbf{A}$

DMD integrates into the QTT framework, maintaining exponentially fine resolution, and offering **extrapolation**, **interpolation**, and **denoising**

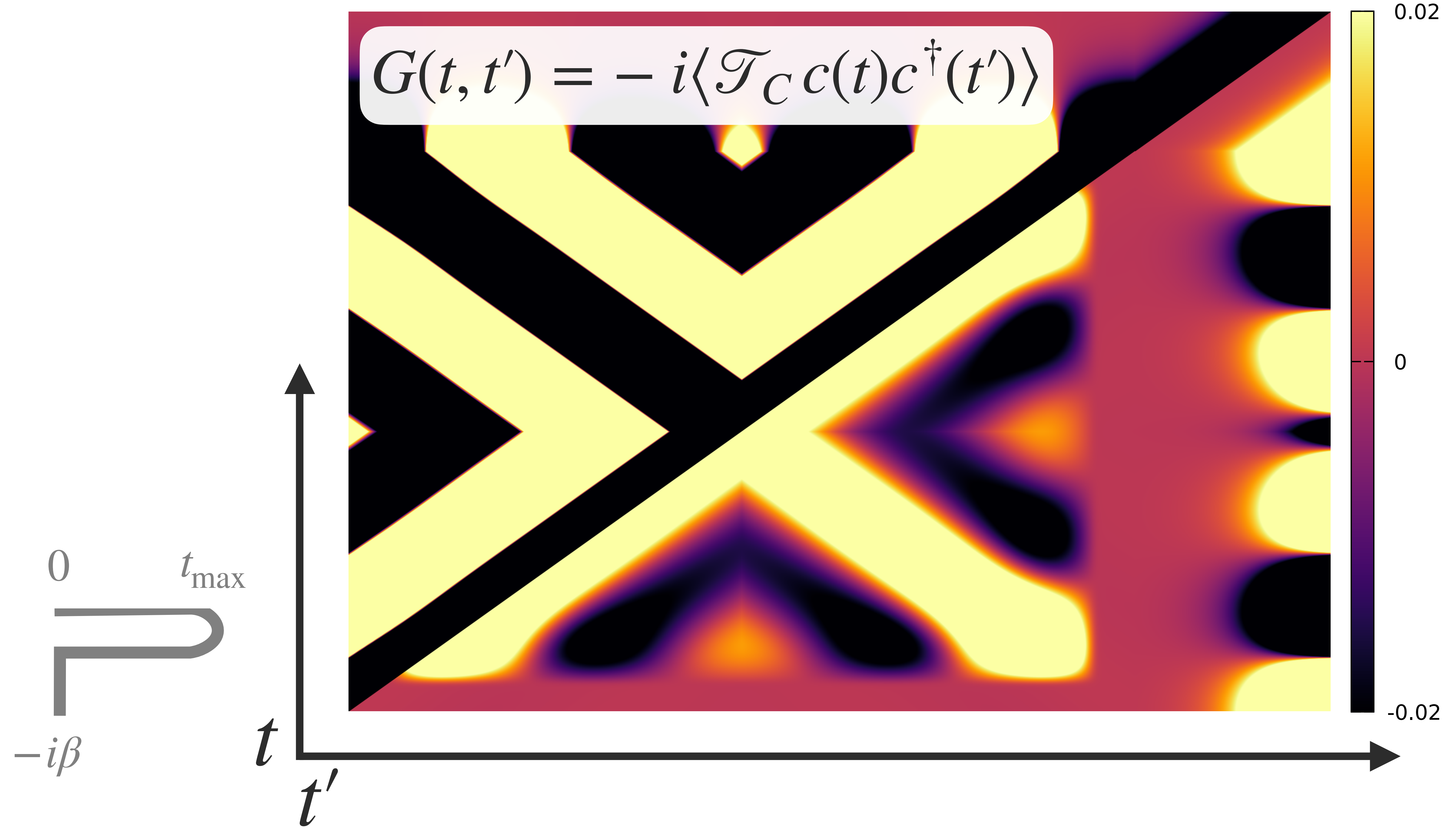
M. Środa et al, arXiv:2509.22177, 2025





H. Aoki et al, RMP 86, 779 (2014)

Nonequilibrium Green's function (NEGF) formalism faces a memory bottleneck



Access to:
✓ single-particle expectation values
✓ photoemission spectrum
✓ energy

Dyson equation

$$G = G_0 + G_0 \star \Sigma \star G$$

$$\int_C d\bar{t}\, \Sigma(t,\bar{t}) G(\bar{t},t') \simeq \sum_{\bar{t}} \Delta\bar{t}\, \Sigma_{t,\bar{t}} G_{\bar{t},t'}$$

convolution = matrix multiplication
need to keep all previous times in memory

Ongoing work to avoid this

SciPost | SciPost Phys. 10, 091 (2021)

Low rank compression in the numerical solution of the nonequilibrium Dyson equation

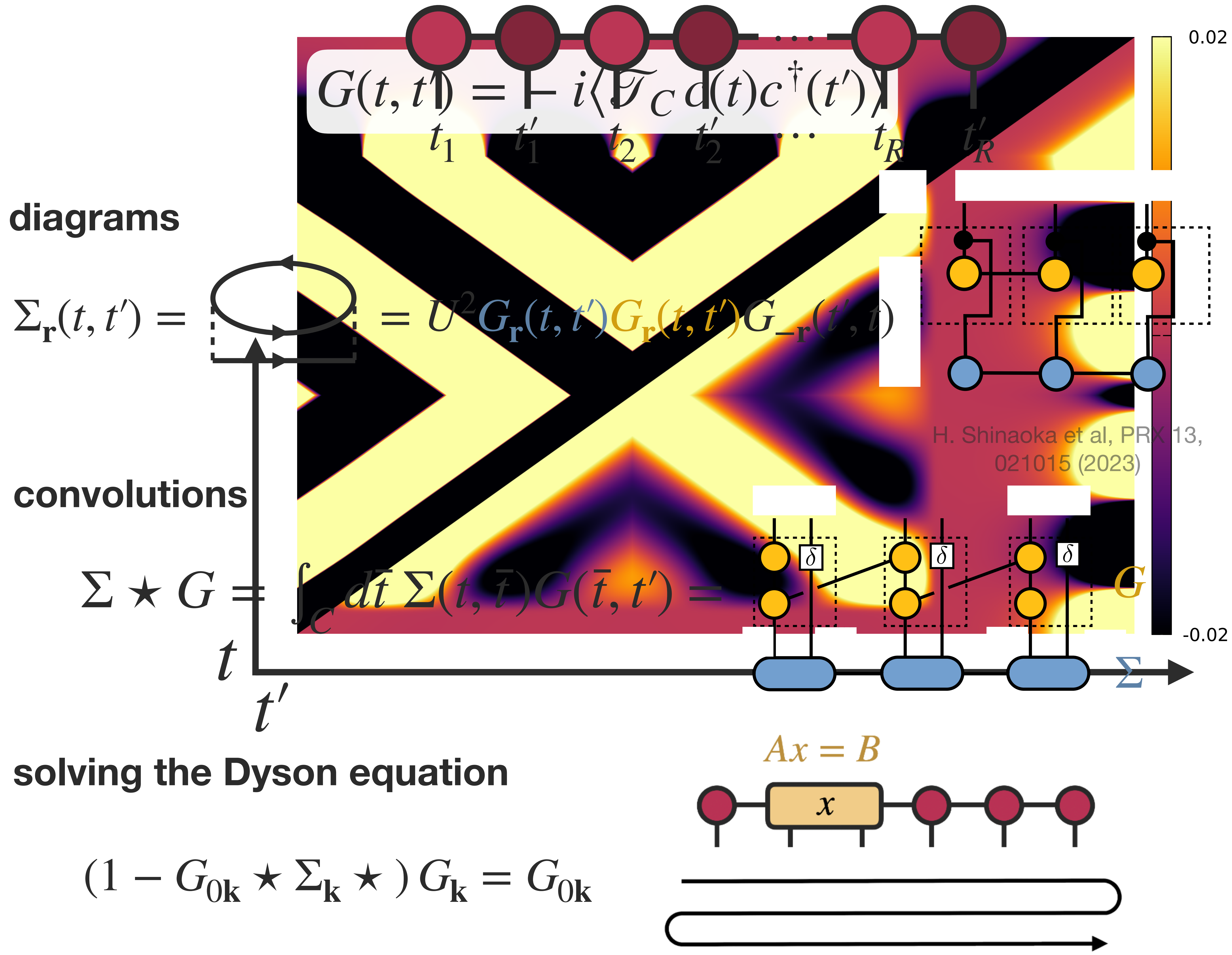
Jason Kaye[1,2] and Denis Golež[2,3,4]

Memory truncated Kadanoff-Baym equations

Christopher Stahl, Nagamalleswararao Dasari, Jiajun Li, Antonio Picano, Philipp Werner, and Martin Eckstein
Phys. Rev. B **105**, 115146 – Published 31 March 2022

...

Quantics tensor trains outcompete conventional matrix-based approaches, but the convergence is not satisfactory

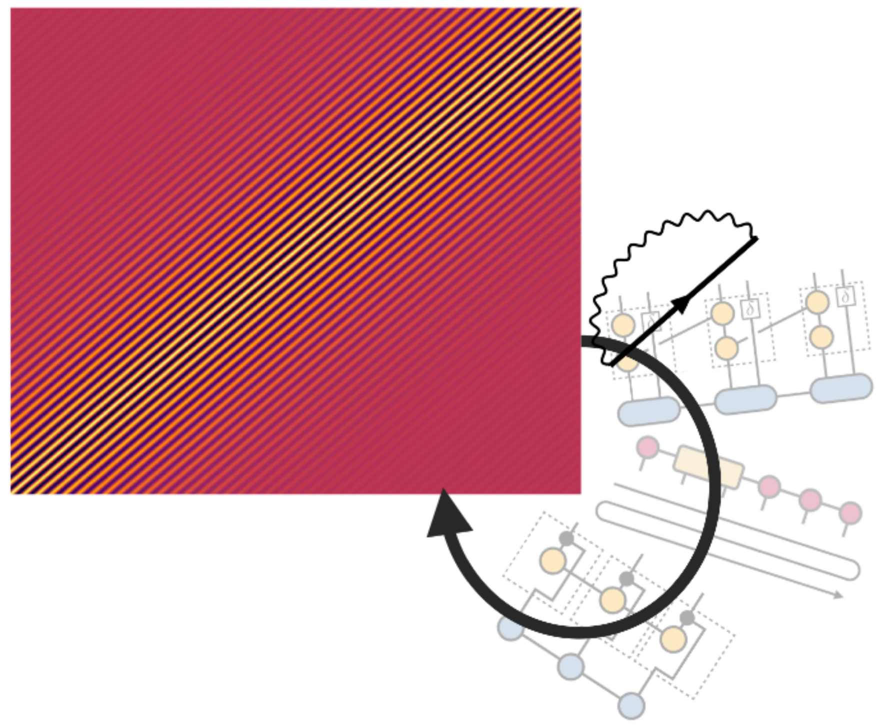


M. Środa et al, arXiv:2412.14032, 2024

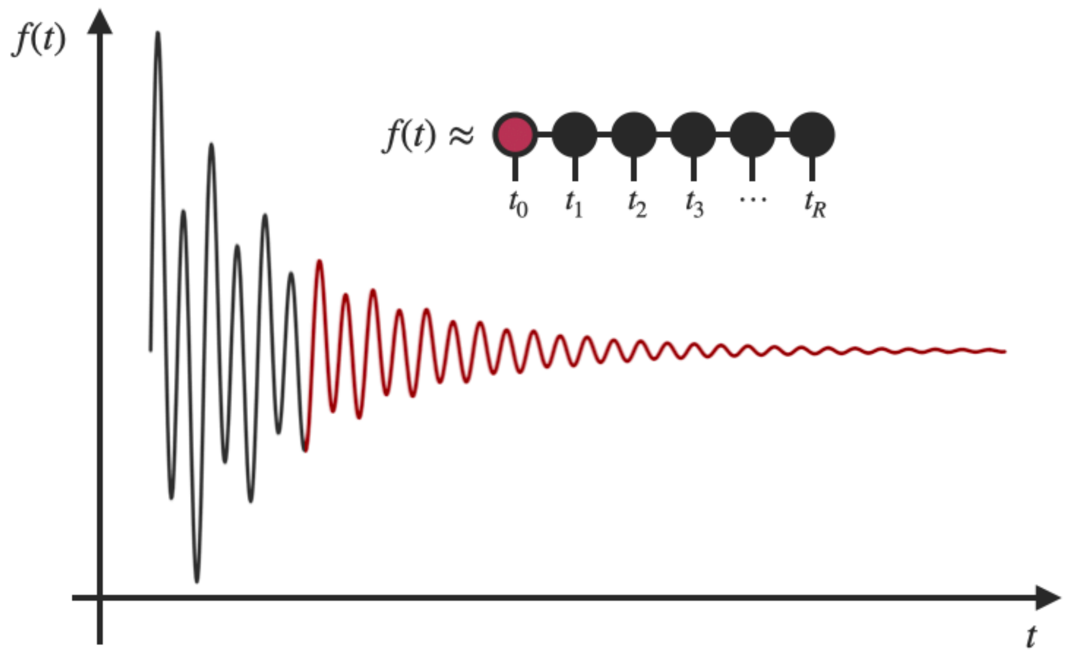
PROBLEM: unstable and slow convergence, difficulty extending $t_{\max}$ and increasing U

SOLUTION: reliable extrapolated initial guess and causality-based solver

Global and causal self-consistency

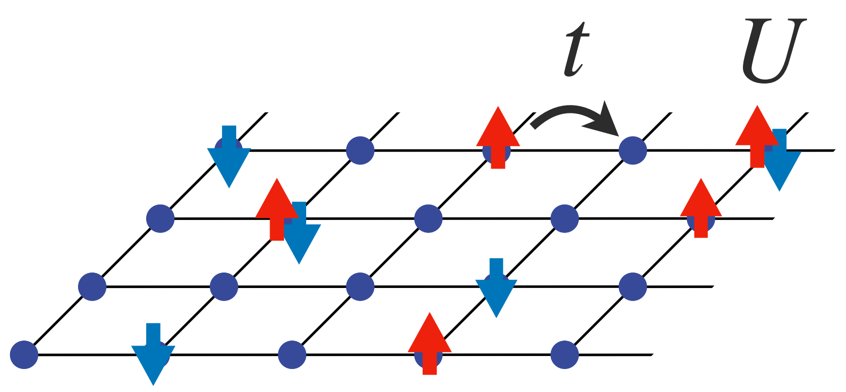


Extrapolating QTTs with dynamic mode decomposition



Results in application to nonequilibrium Green’s functions

$$\Sigma = iGW$$



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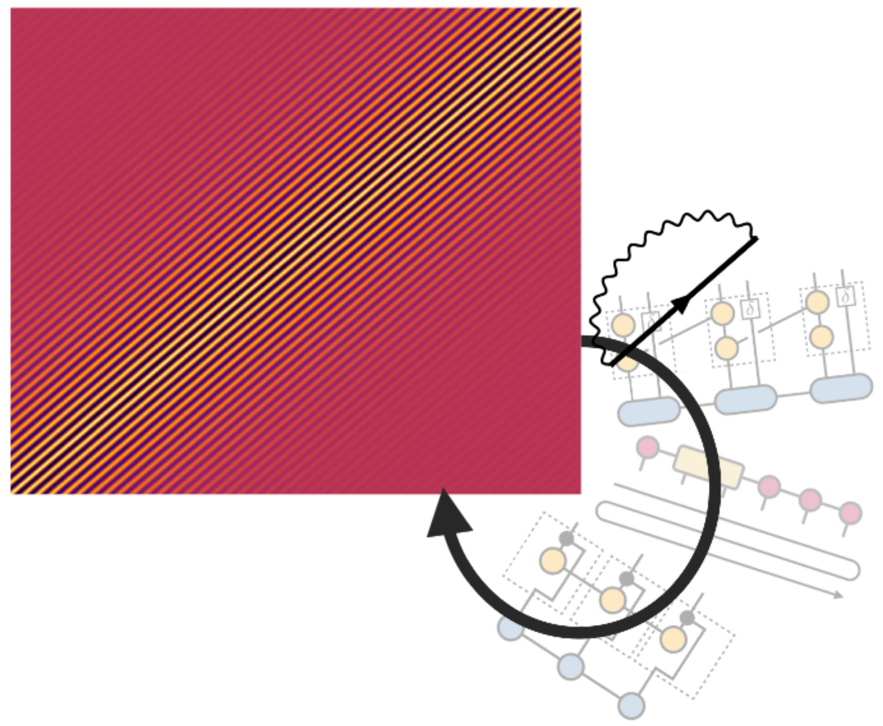

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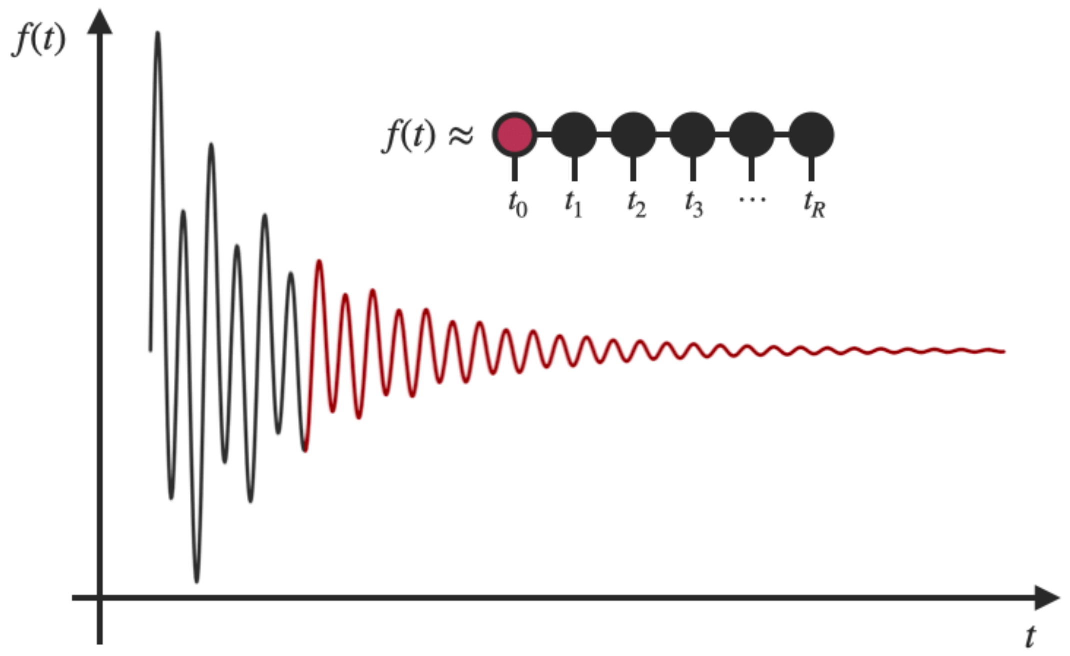

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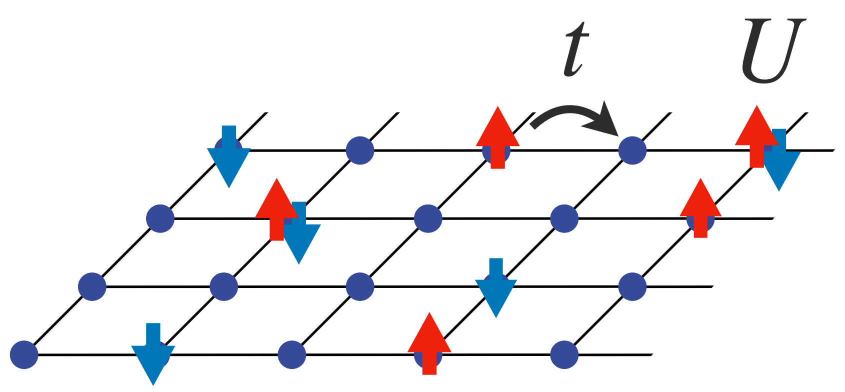


Simplest solver uses a global update which suffers from convergence issues

Take ansatz $G_{\mathbf{k}}(t,t')$

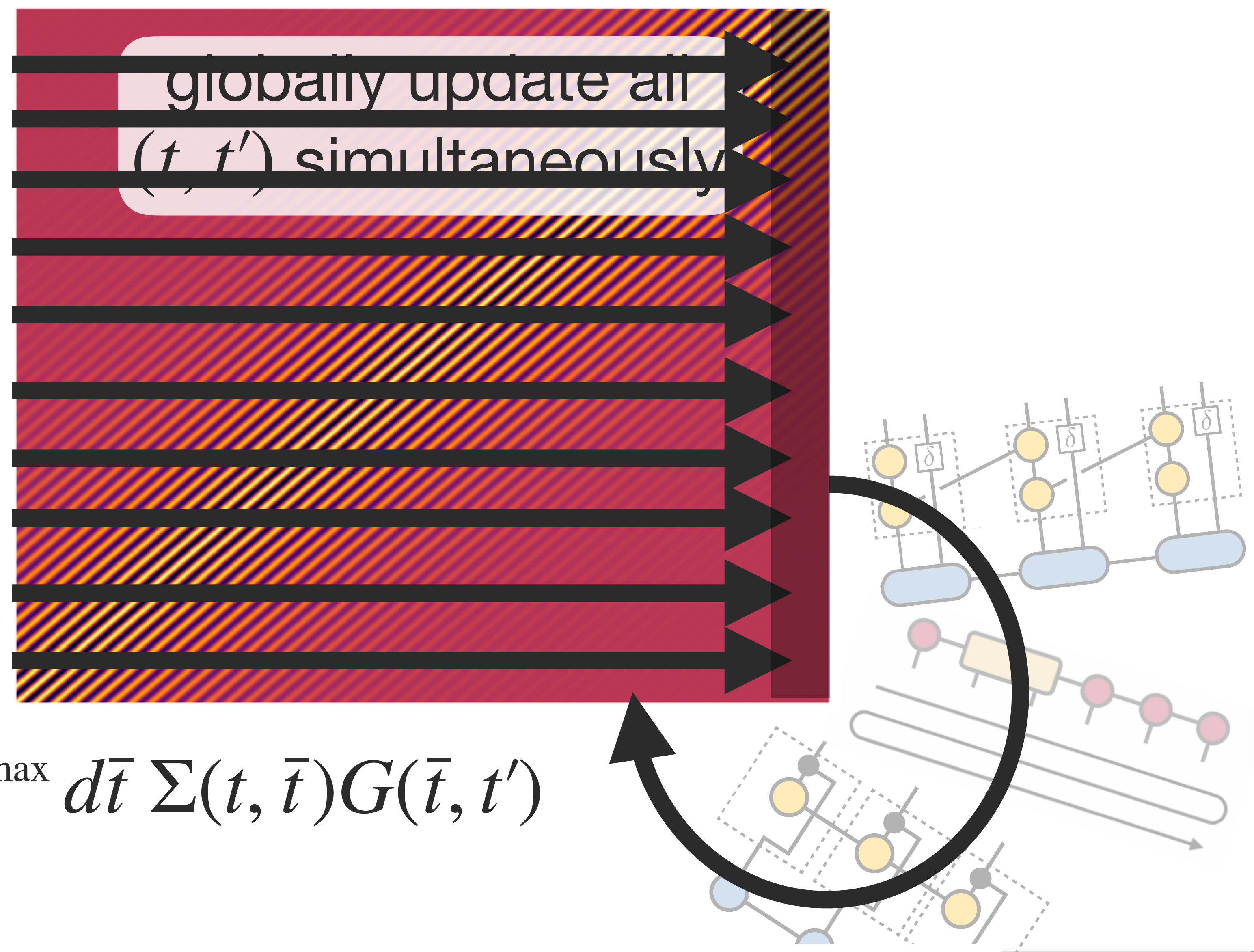
Update by solving

$$(1 - G_{0\mathbf{k}} \star \Sigma_{\mathbf{k}}[G_{\mathbf{k}}^{(n-1)}] \star)\, G_{\mathbf{k}}^{(n)} = G_{0\mathbf{k}}$$

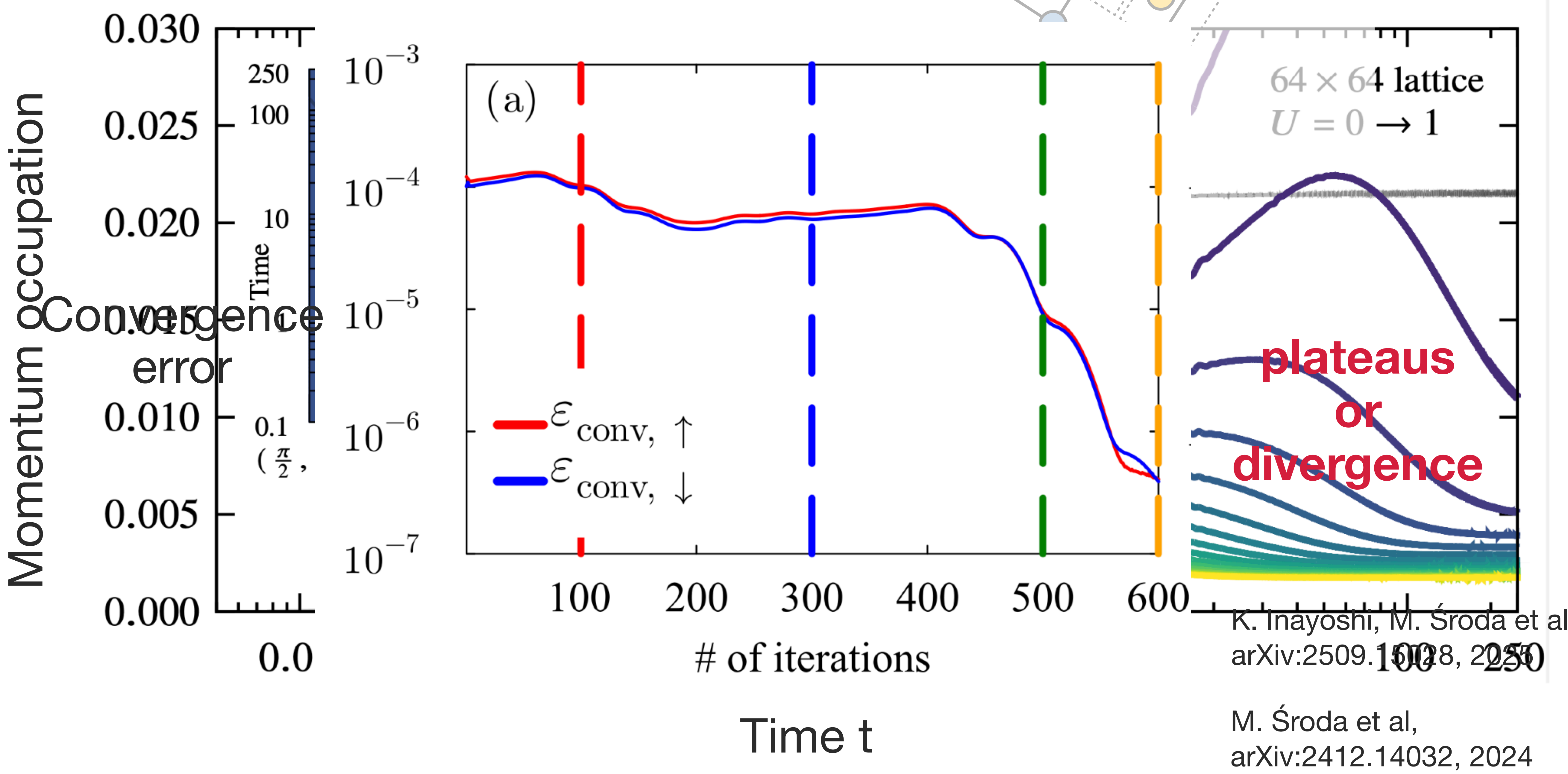
which defines *the new* as a functional of *the old*, $G_{\mathbf{k}}^{(n)}[G_{\mathbf{k}}^{(n-1)}]$

look for fixed point

$$G_{\mathbf{k}}^{(n)}[G_{\mathbf{k}}^{(n-1)}] = G_{\mathbf{k}}^{(n-1)}$$



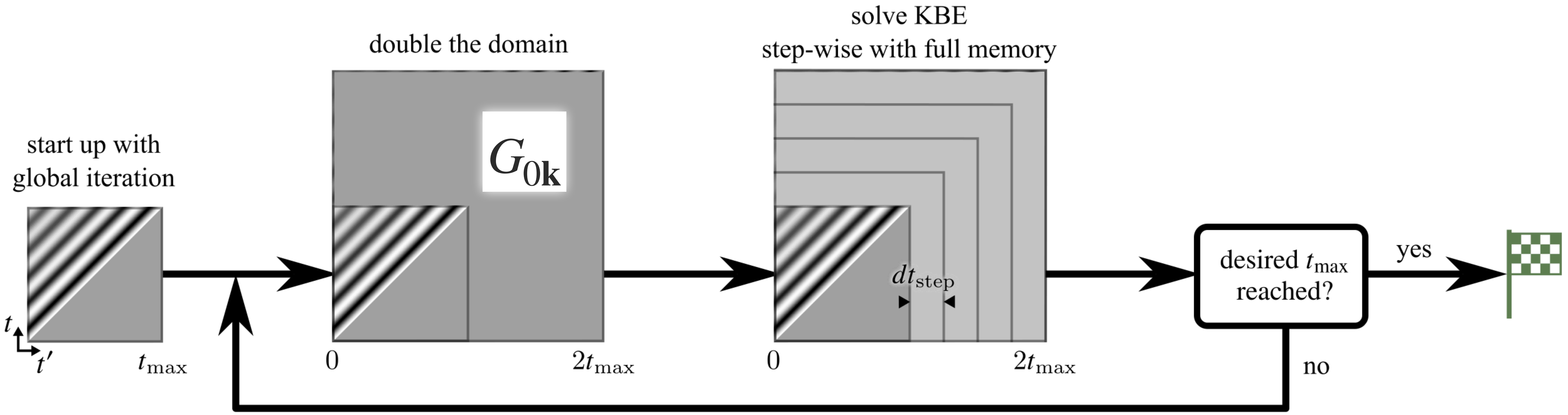
$$\int_0^{t_{\max}} d\bar{t}\; \Sigma(t,\bar{t})G(\bar{t},t')$$

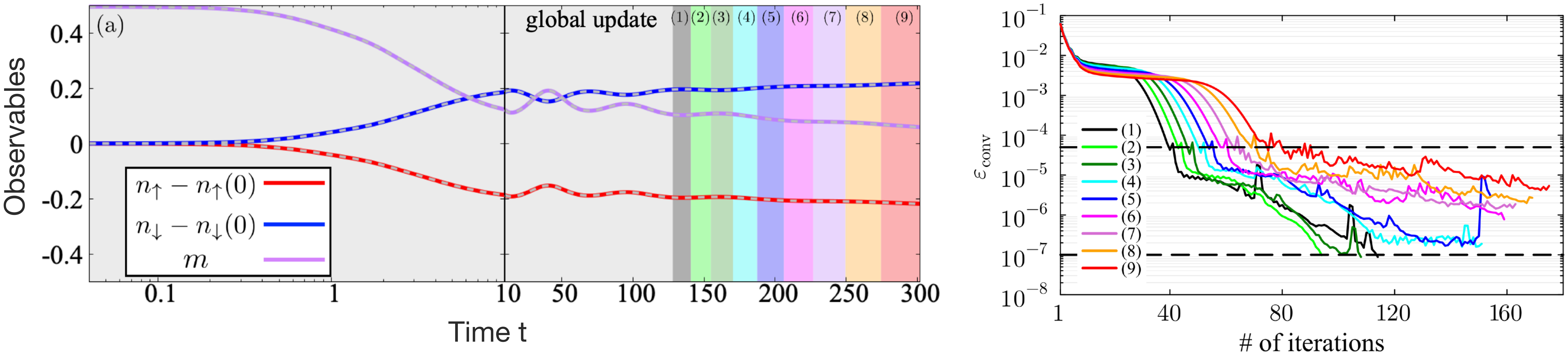


K. Inayoshi, M. Środa et al, arXiv:2509.15028, 2025

M. Środa et al, arXiv:2412.14032, 2024

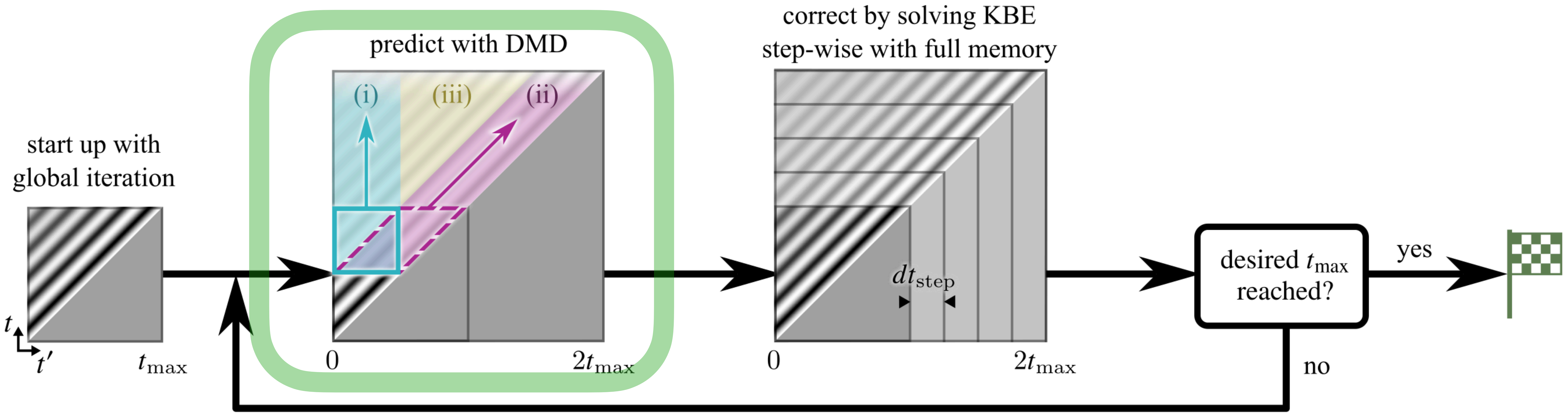
Enforcing causality makes convergence more stable

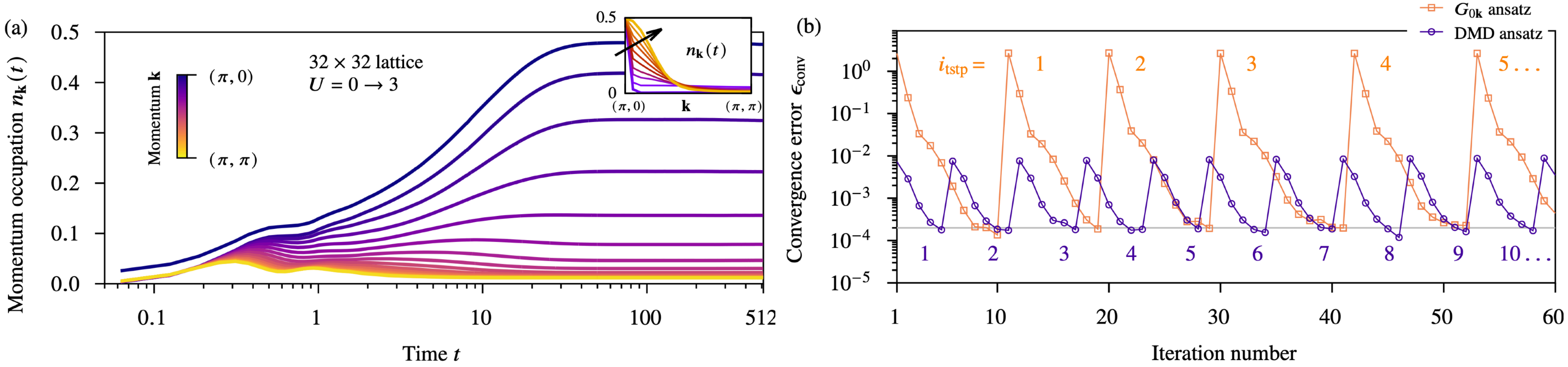




K. Inayoshi, M. Środa et al, arXiv:2509.15028, 2025

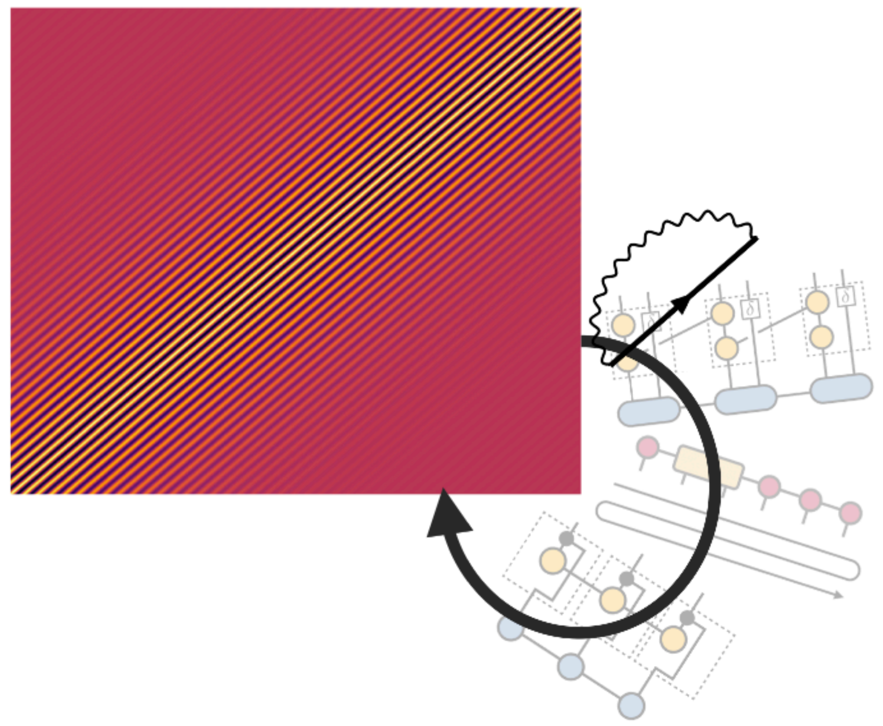
Using DMD extrapolation as initial guess gives stable, predictable and accelerated convergence



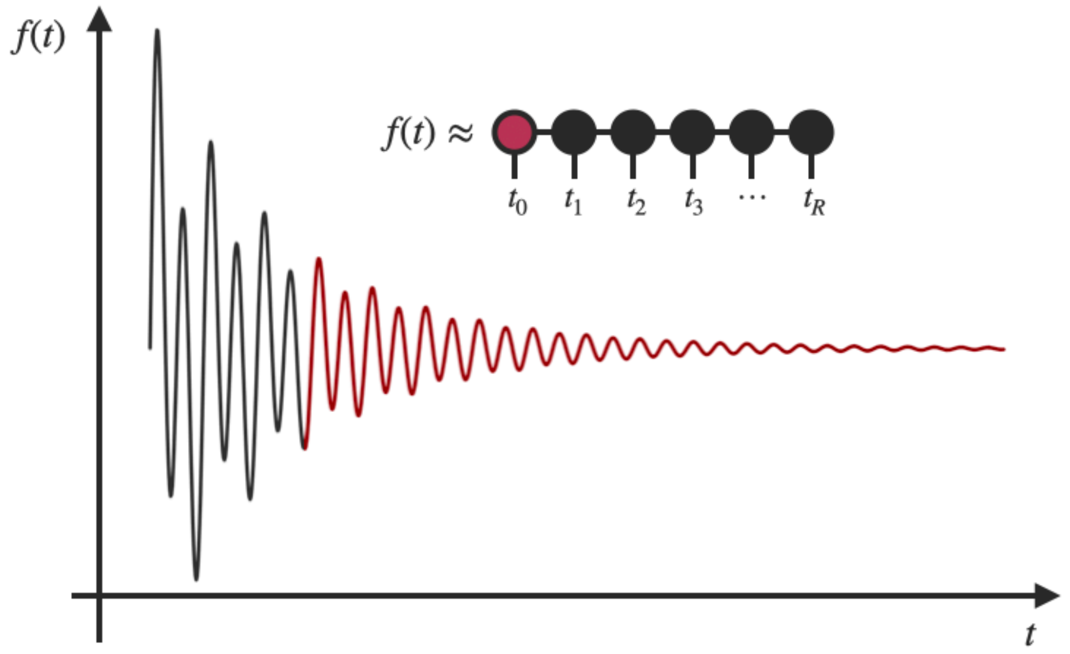


M. Środa et al, arXiv:2509.22177, 2025

Global and causal self-consistency



Extrapolating QTTs with dynamic mode decomposition



Results in application to nonequilibrium Green’s functions

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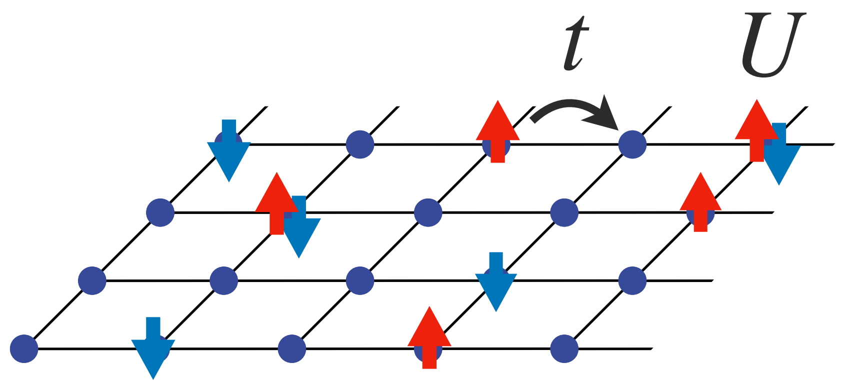
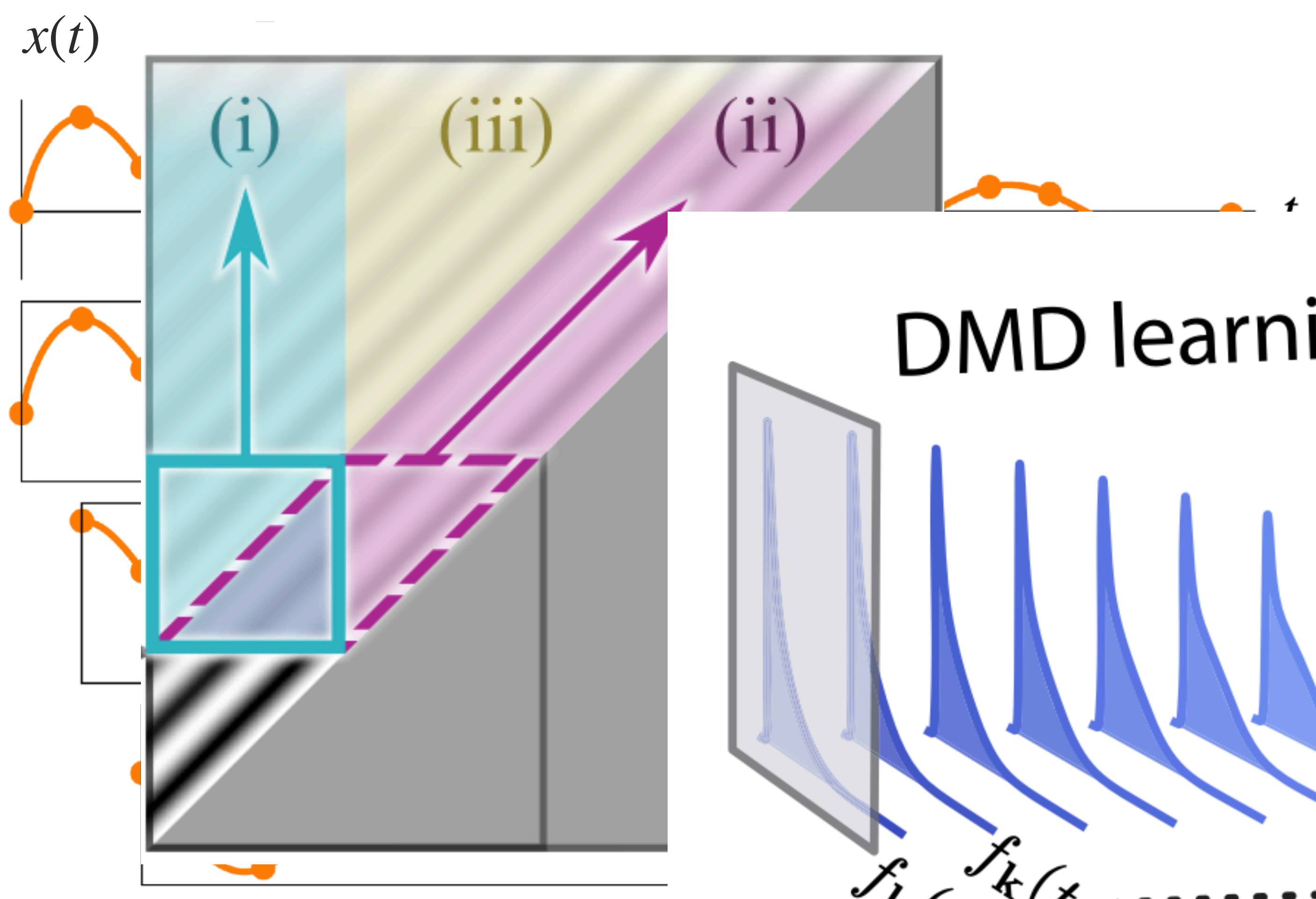


Let’s recall the matrix-based DMD

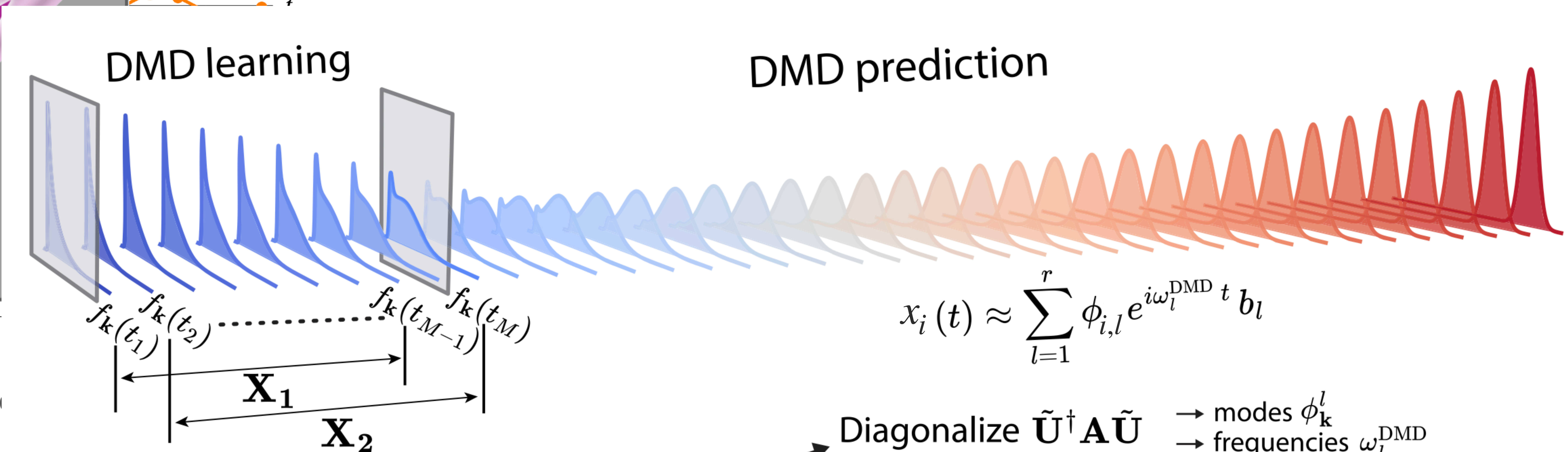
$$\begin{array}{c} \text{time points} \rightarrow \\ \text{observables} \downarrow \end{array} \quad \mathbf{X} = \begin{pmatrix} \vdots & \vdots & & \vdots & & \vdots \\ x_i(0) & x_i(dt) & \cdots & x_i(m\,dt) & \cdots & x_i(t_{\max}) \\ \vdots & \vdots & & \vdots & & \vdots \end{pmatrix} \longrightarrow$$

$$\mathbf{X}_1 = \begin{pmatrix} \vdots & \vdots & & \vdots & & \vdots \\ x_i(0) & x_i(dt) & \cdots & x_i(m\,dt) & \cdots & x_i(t_{\max} - dt) \\ \vdots & \vdots & & \vdots & & \vdots \end{pmatrix}$$

$$\mathbf{X}_2 = \begin{pmatrix} \vdots & \vdots & & \vdots & & \vdots \\ x_i(dt) & x_i(2dt) & \cdots & x_i((m+1)\,dt) & \cdots & x_i(t_{\max}) \\ \vdots & \vdots & & \vdots & & \vdots \end{pmatrix}$$



Kaneko et al., PRR 7, 013085 (2(



$$x_i(t) \approx \sum_{l=1}^{r} \phi_{i,l} e^{i\omega_l^{\mathrm{DMD}} t} b_l$$

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{A}\mathbf{x}(t) \longrightarrow \mathbf{X_2} = \mathbf{A}\mathbf{X_1}$$

$$\mathbf{A} = \mathbf{X}_2\mathbf{X}_1^{-1}$$

SVD: $\mathbf{X_1} \approx \tilde{\mathbf{U}}\tilde{\mathbf{\Sigma}}\tilde{\mathbf{V}}^\dagger$

(full operator would be $\mathbf{A} = \mathbf{X}_2\tilde{\mathbf{V}}\tilde{\mathbf{\Sigma}}^{-1}\tilde{\mathbf{U}}^\dagger$)

Diagonalize $\tilde{\mathbf{U}}^\dagger\mathbf{A}\tilde{\mathbf{U}}$ → modes $\phi_{\mathbf{k}}^l$ → frequencies ω_l^{DMD}

mode amplitudes b_l from $f_{\mathbf{k}}(t_1)$

I. Maliyov et al., npj Computational Materials 10, 123 (2024)

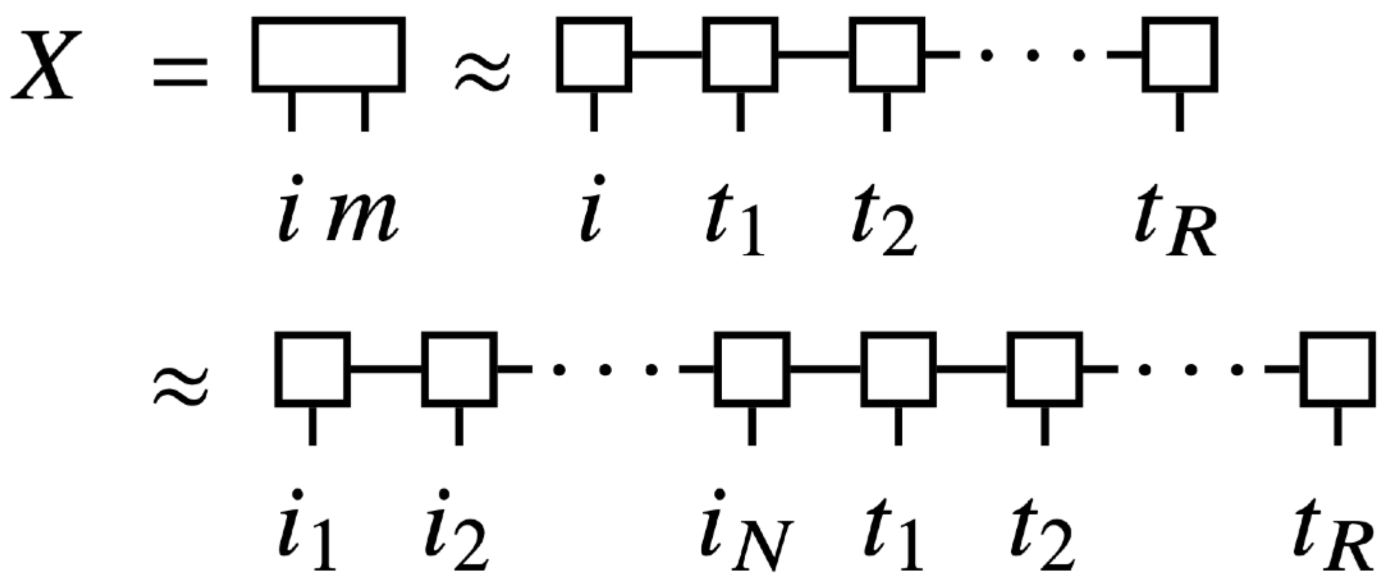
Let's translate DMD into the QTT language

time points

observables

$$X = \begin{pmatrix} \vdots & \vdots & & \vdots & & \vdots \\ x_i(0) & x_i(dt) & \cdots & x_i\big(m\,dt\big) & \cdots & x_i(t_{\max}) \\ \vdots & \vdots & & \vdots & & \vdots \end{pmatrix}$$

Assume **quantics** encoding $m = t/dt = [t_1, \ldots, t_R]_2$



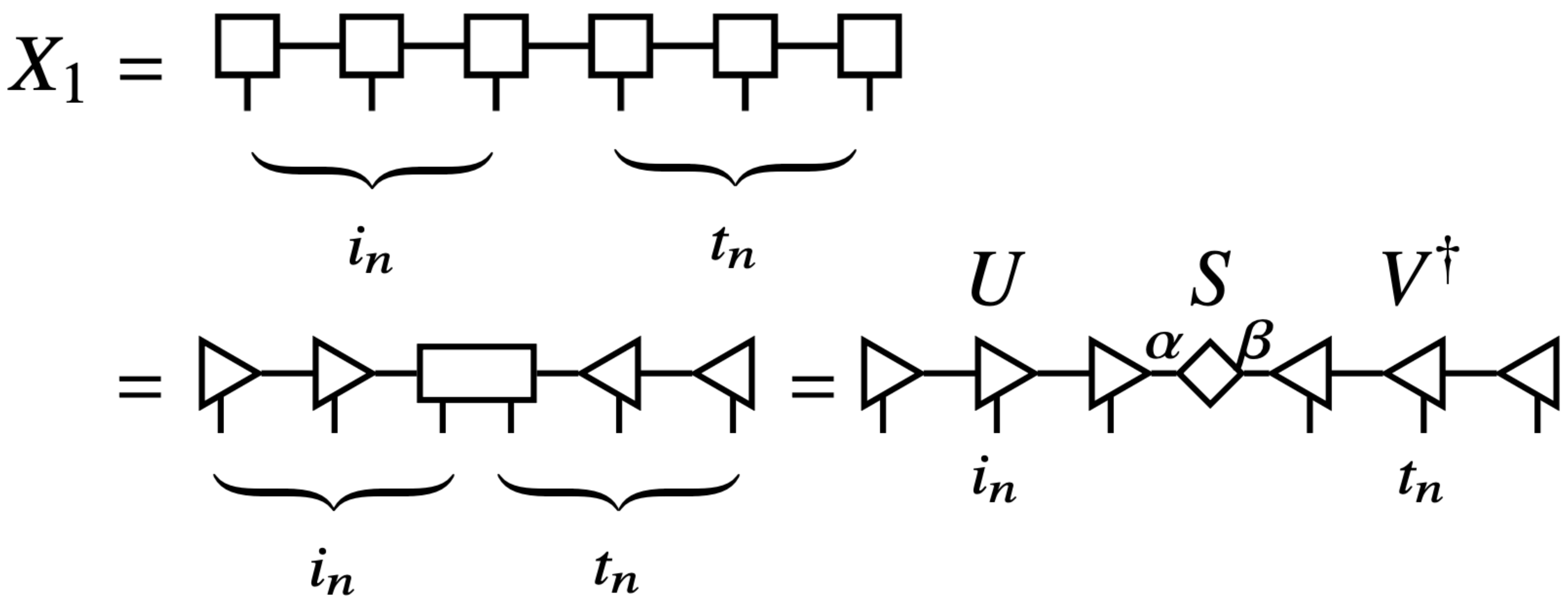
and **assume i also factorizes** in some way.

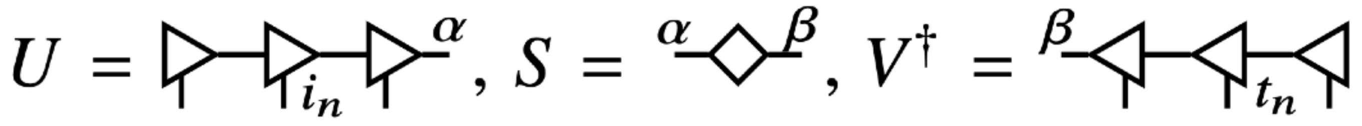
X_1, X_2 obtained by a shift with MPO
(and zeroing of the last col)

We aim to find the operator

$$AX_1 = X_2, \quad A = X_2 X_1^{-1}$$

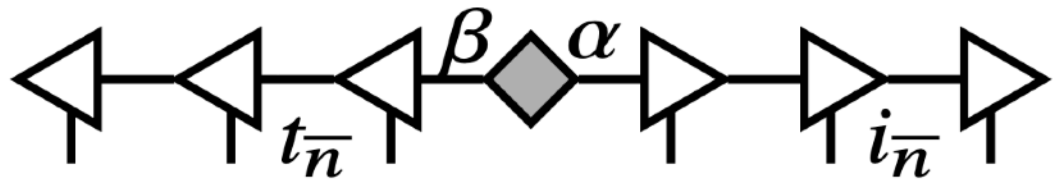
so **we need SVD of X_1** to calculate the pseudoinverse



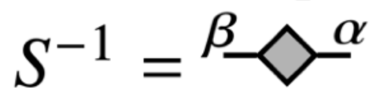


The pseudoinverse thus is the usual

$$X_1^{-1} = VS^{-1}U^\dagger =$$



Klus et al., Nonlinearity
31, 3359–3380 (2018)

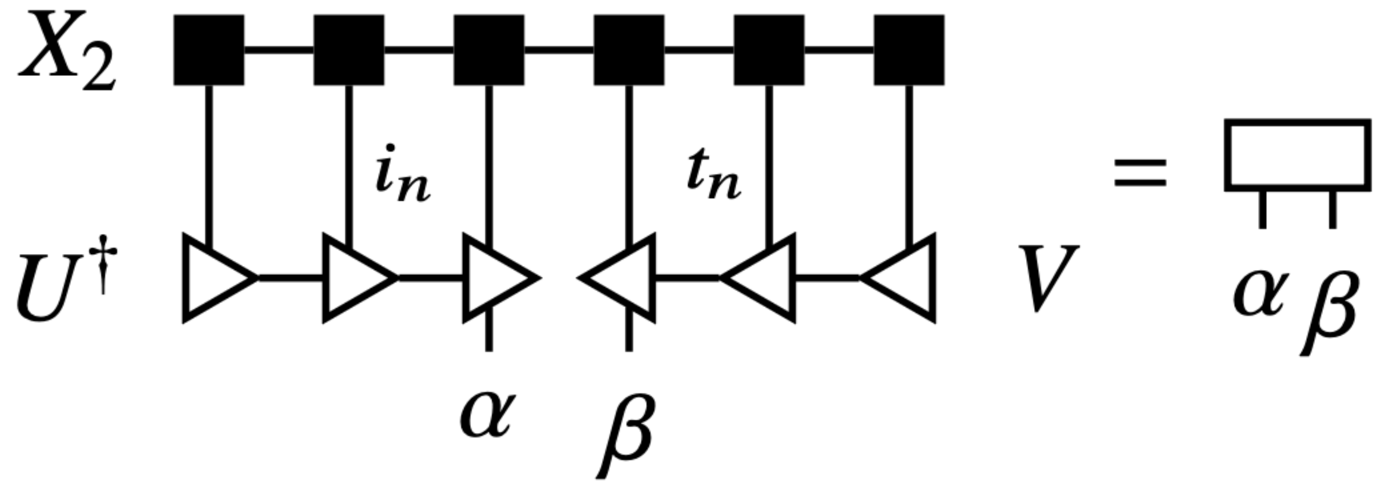


Define **rank-r approximation** to the full operator A

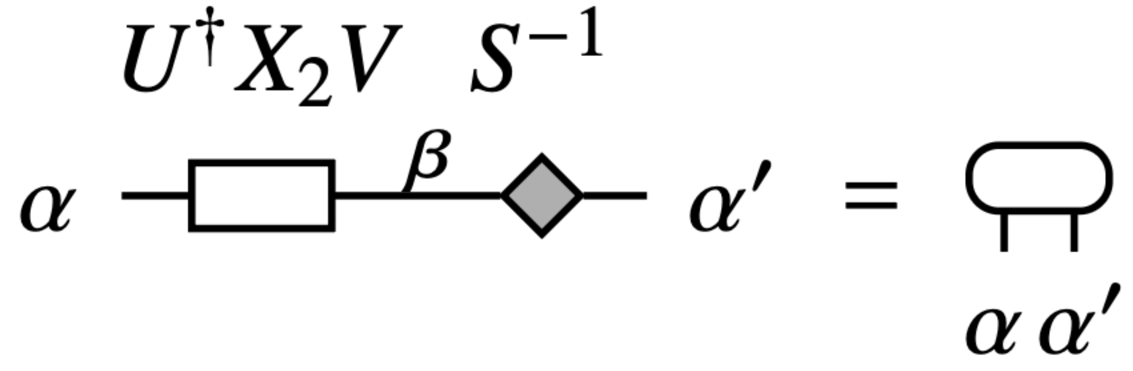
$$\tilde{A} \equiv U^\dagger A U = U^\dagger X_2 V S^{-1}$$

Diagrammatically,

$U^\dagger X_2 V =$

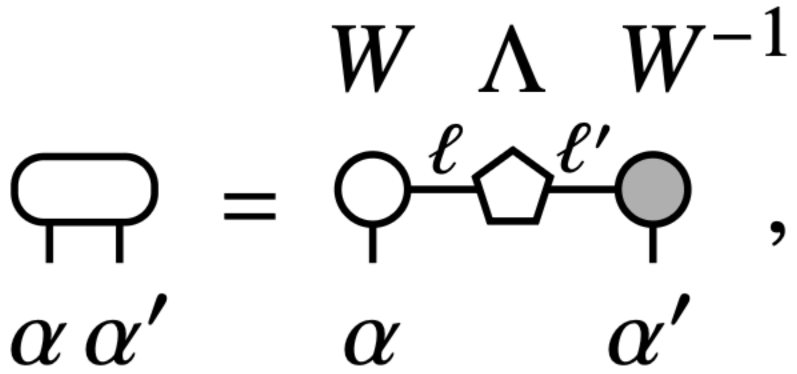


$\tilde{A} =$



Eigendecompose with a std dense-matrix algorithm

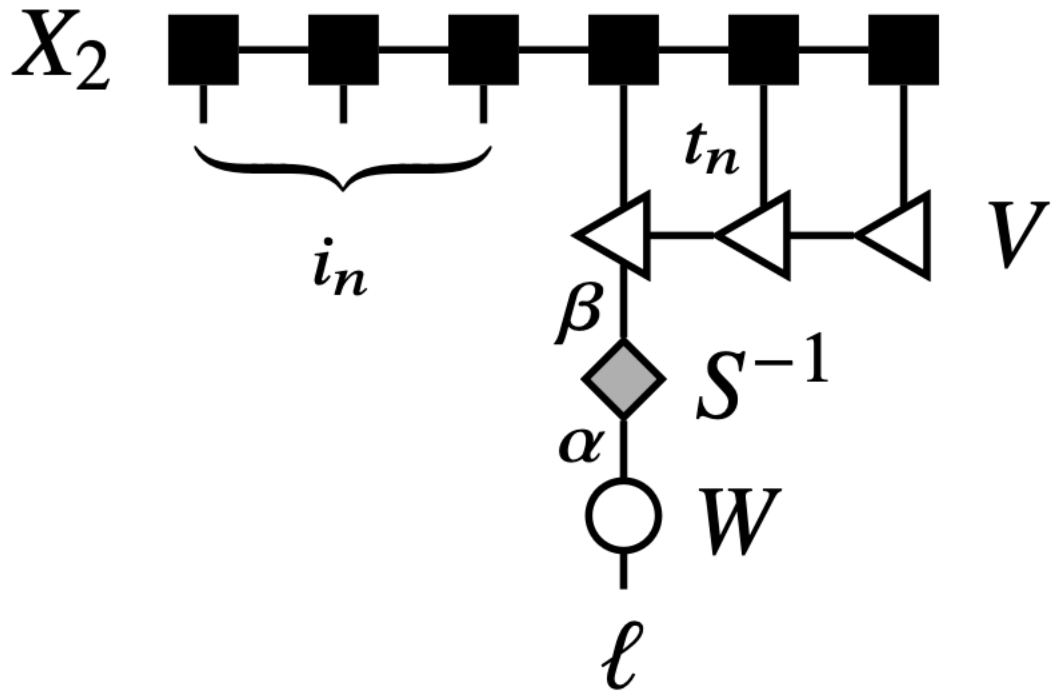
$\tilde{A} =$



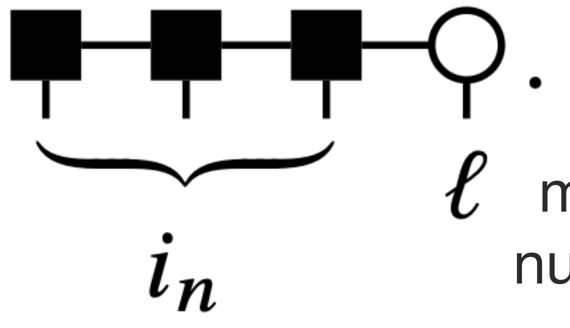
Matrices Λ, W contain approximate eigenvalues and eigenvectors in the reduced space.

The dynamic modes are the eigenvectors of full A in the original space, hence transforming back

$\Phi = X_2 V S^{-1} W =$



$=$



mode number

temporal dependence $\Rightarrow$ eigenvalue λ_ℓ

"spatial" dependence

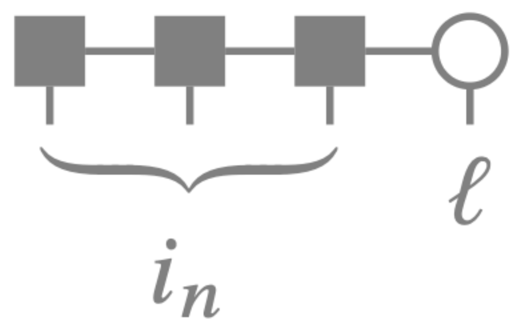
The **dynamic mode decomposition** is a **spatio-temporal superposition** of the modes Φ with amplitudes b,

$$X \approx \Phi \Lambda^m b = \Phi\,\mathrm{diag}(|\lambda_\ell|^m e^{i\omega_\ell m})\, b,$$

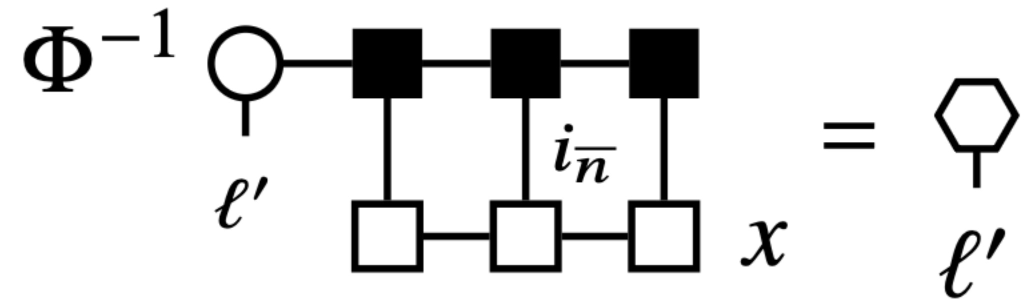
$$m = t/dt = [t_1, \ldots, t_R]_2$$

Amplitudes are fitted to the initial condition x

$$b = \Phi^{-1} x, \qquad \Phi =$$



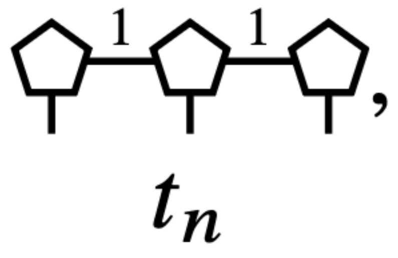
$b =$



Finally, we prepare Λ^m as a single QTT representing all m powers.

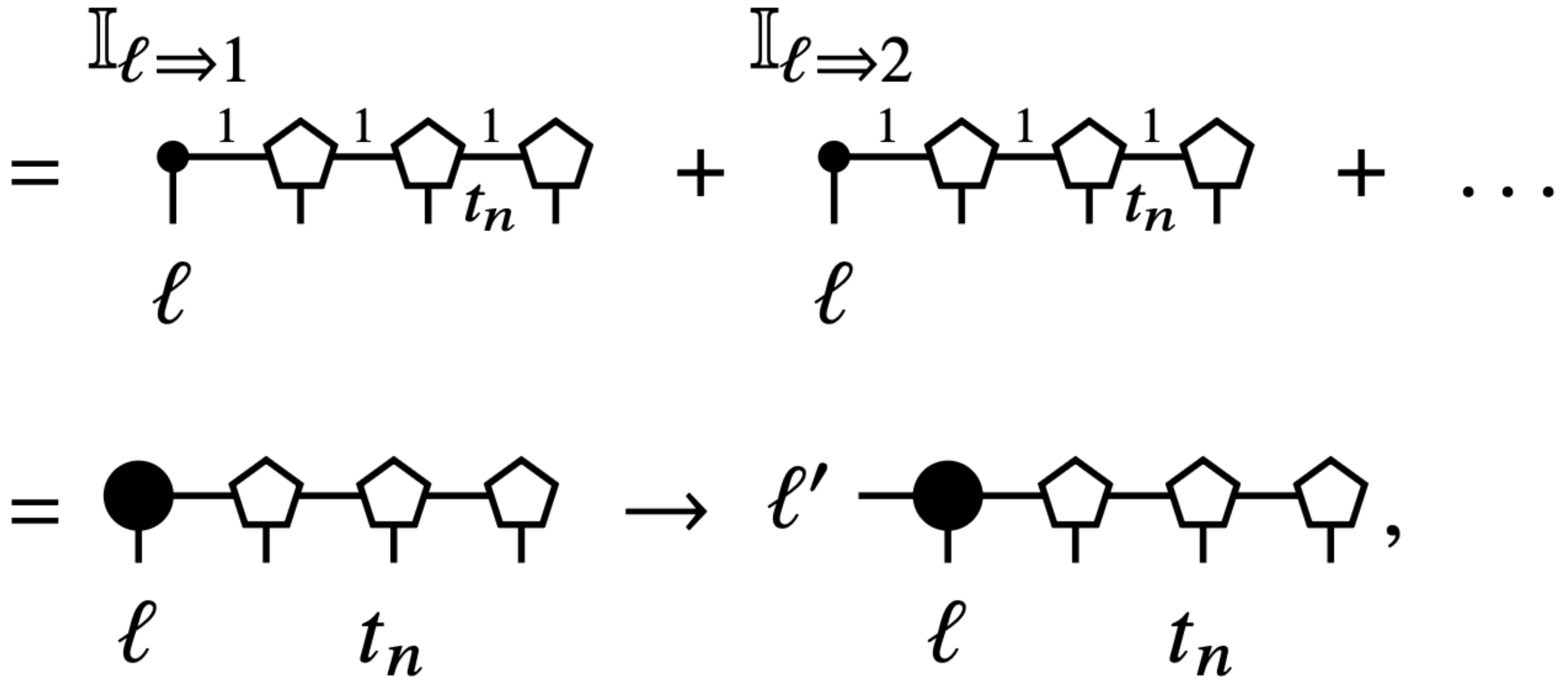
For a single eigenvalue λ, we note that

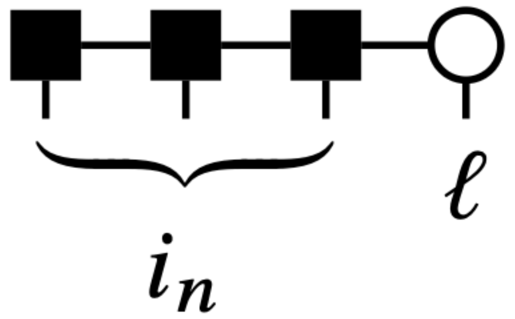
$$\lambda^m = e^{m \ln \lambda} = e^{[t_1, \ldots, t_R]_2 \ln \lambda} = \prod_{n=1}^{R} e^{2^{R-n} t_n \ln \lambda} =$$

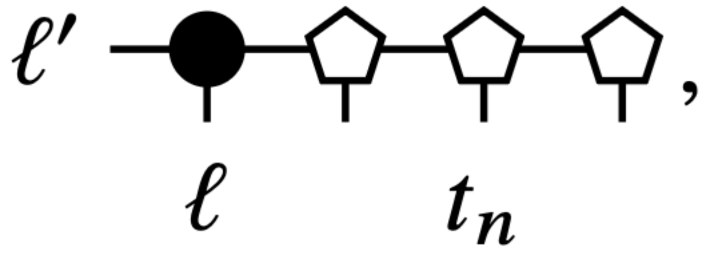


We repeat the above for each λ, tag each QTT with a dummy tensor, and sum

$\Lambda^m =$



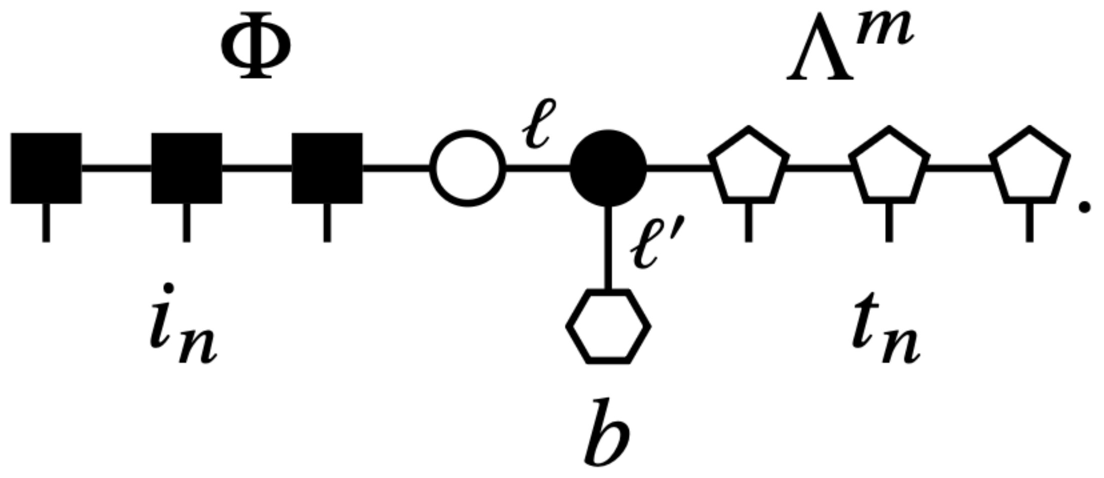
We have all the ingredients: $\Phi =$ 

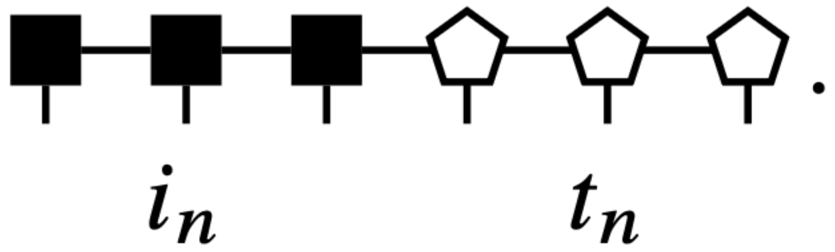
$\Lambda^m =$ 

$b =$ 

So we perform the final contraction:

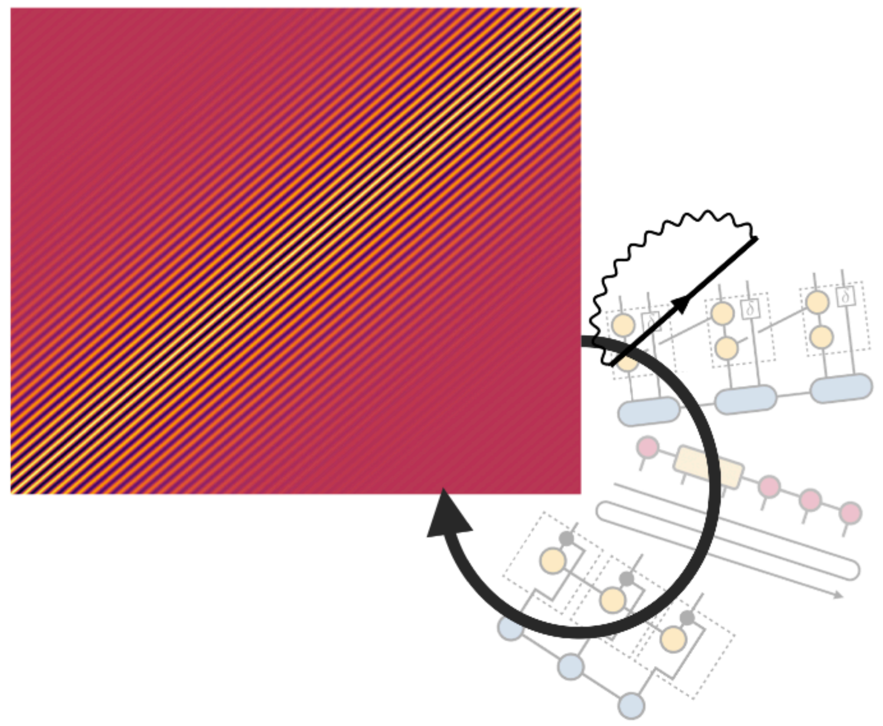
$$X \approx \Phi \Lambda^m b = \Phi\, \mathrm{diag}(|\lambda_\ell|^m e^{i\omega_\ell m})\, b,$$

$X \approx$ 

$=$ 

✓ "recompression"
✓ denoising (set cutoff appropriately in initial SVD of X_1)
✓ extrapolation (add coarse tensor in Λ^m)
✓ interpolation (add fine tensor in Λ^m)
✓ DMD is general (not only time dynamics, no smoothness requirement)

Global and causal self-consistency



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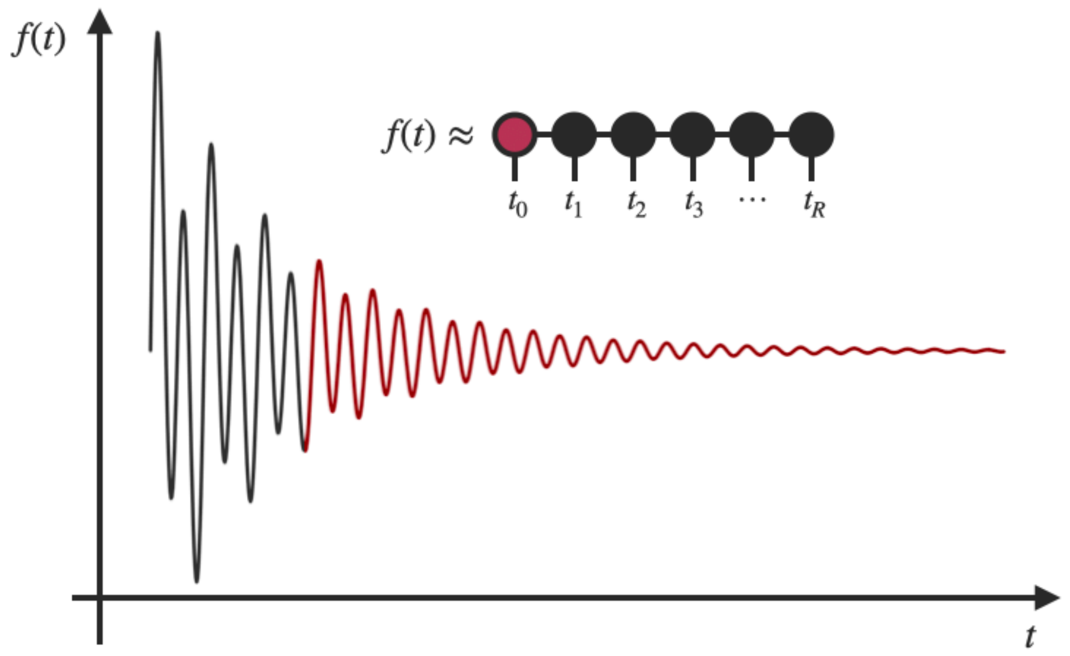

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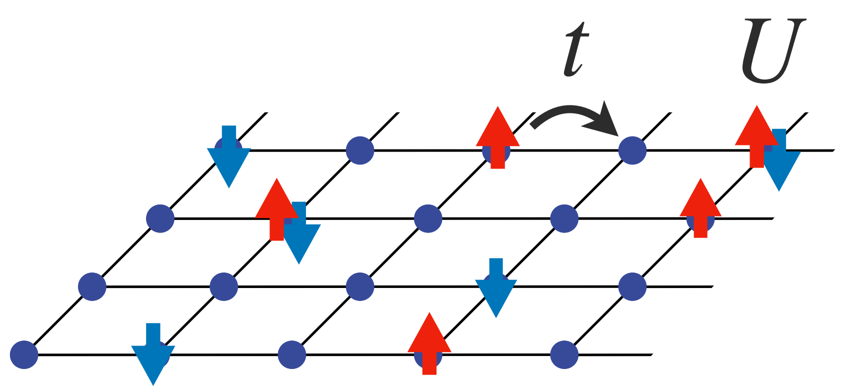
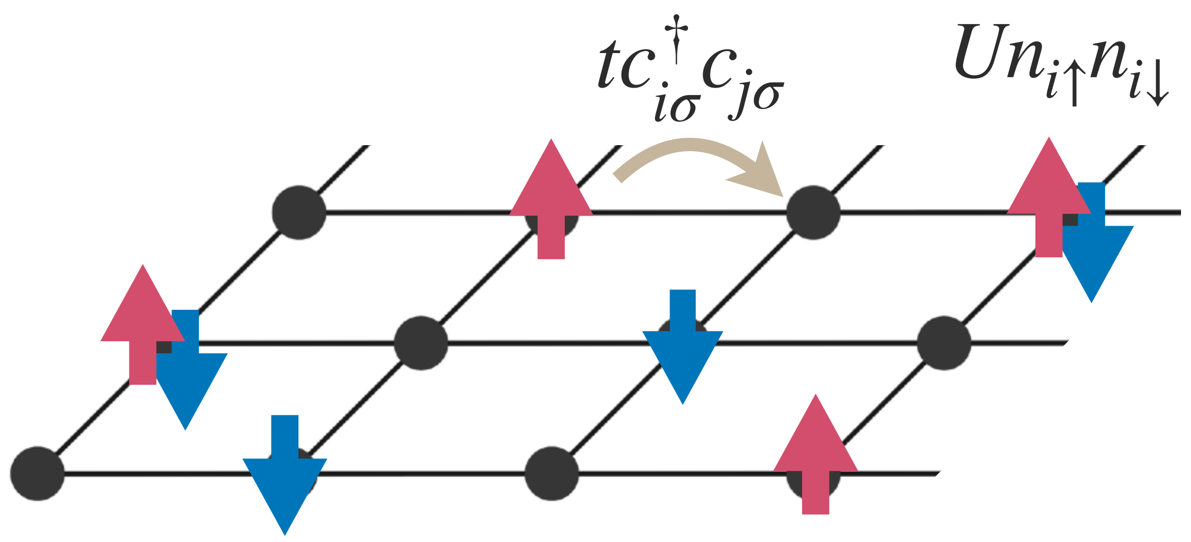
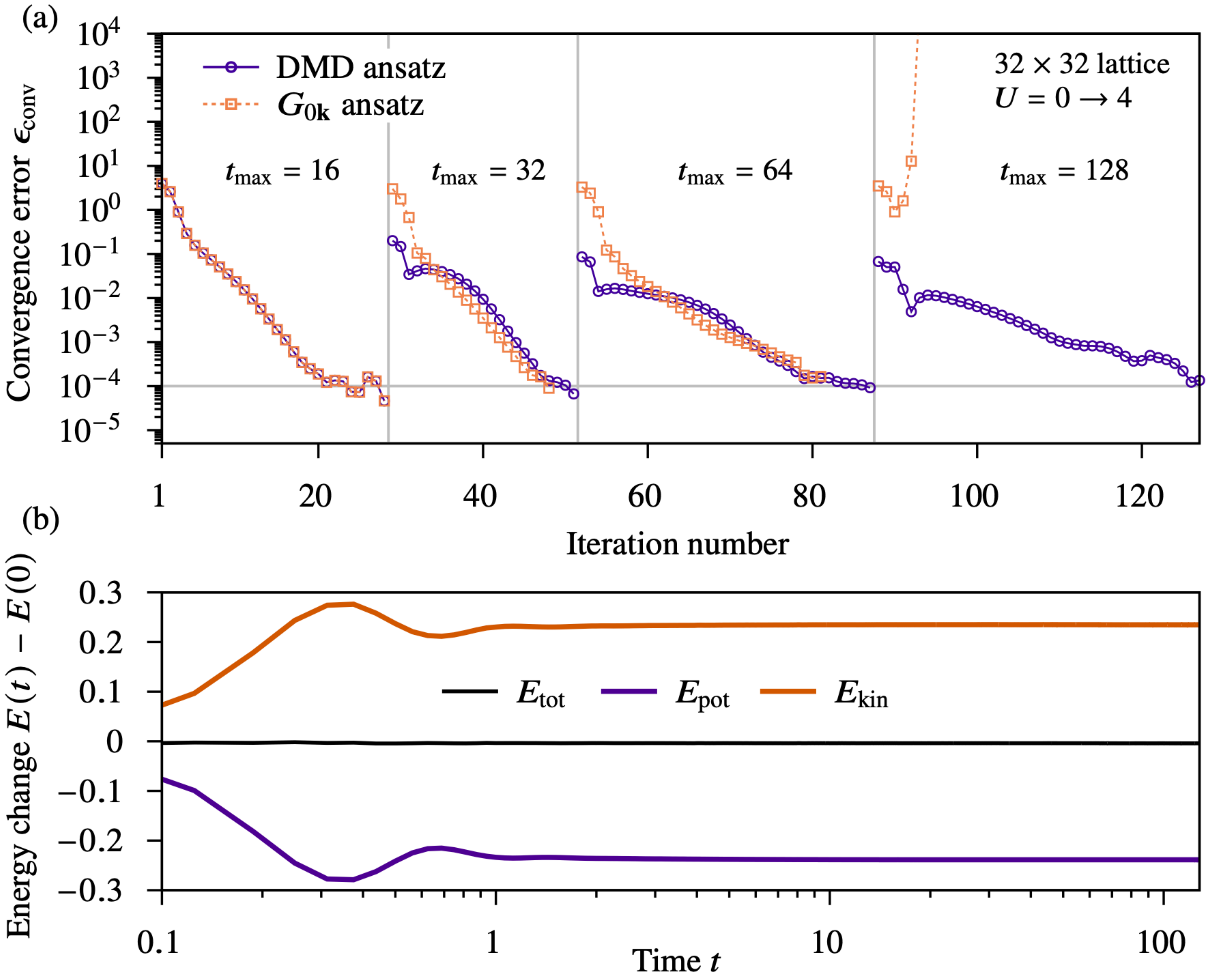


DMD guess stabilizes convergence

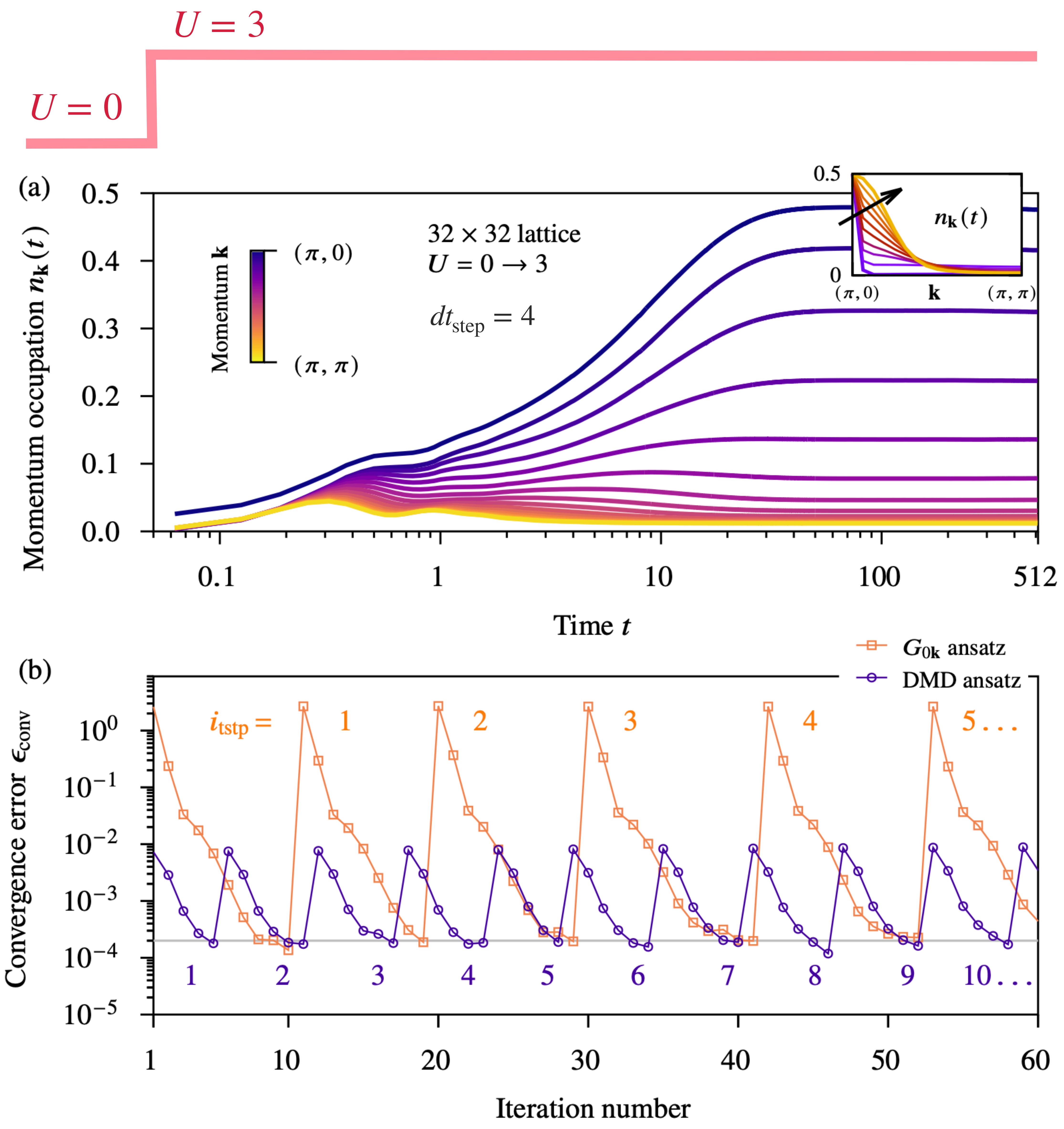
Hubbard model at half-filling



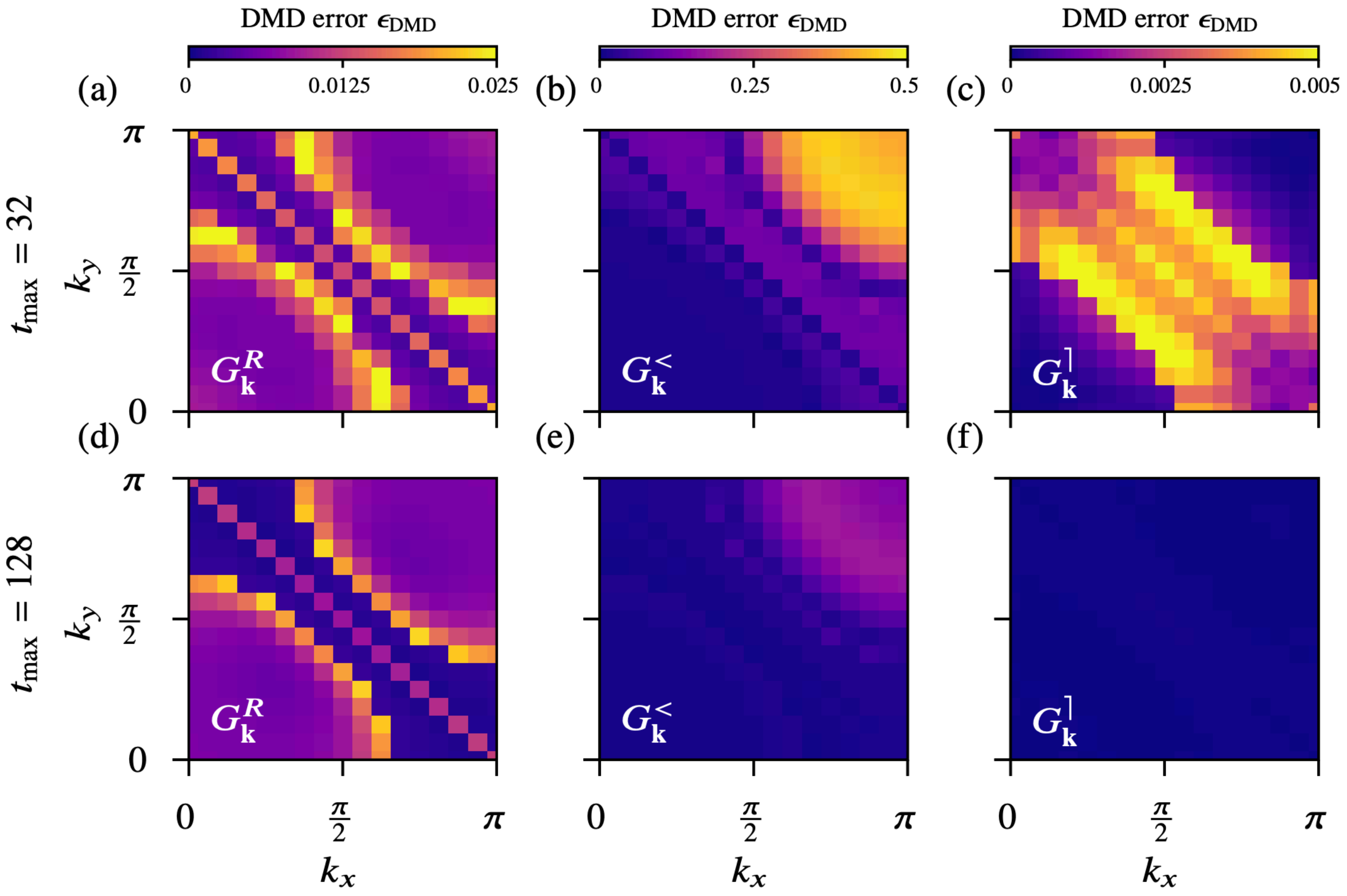
$$\Sigma = iGW$$



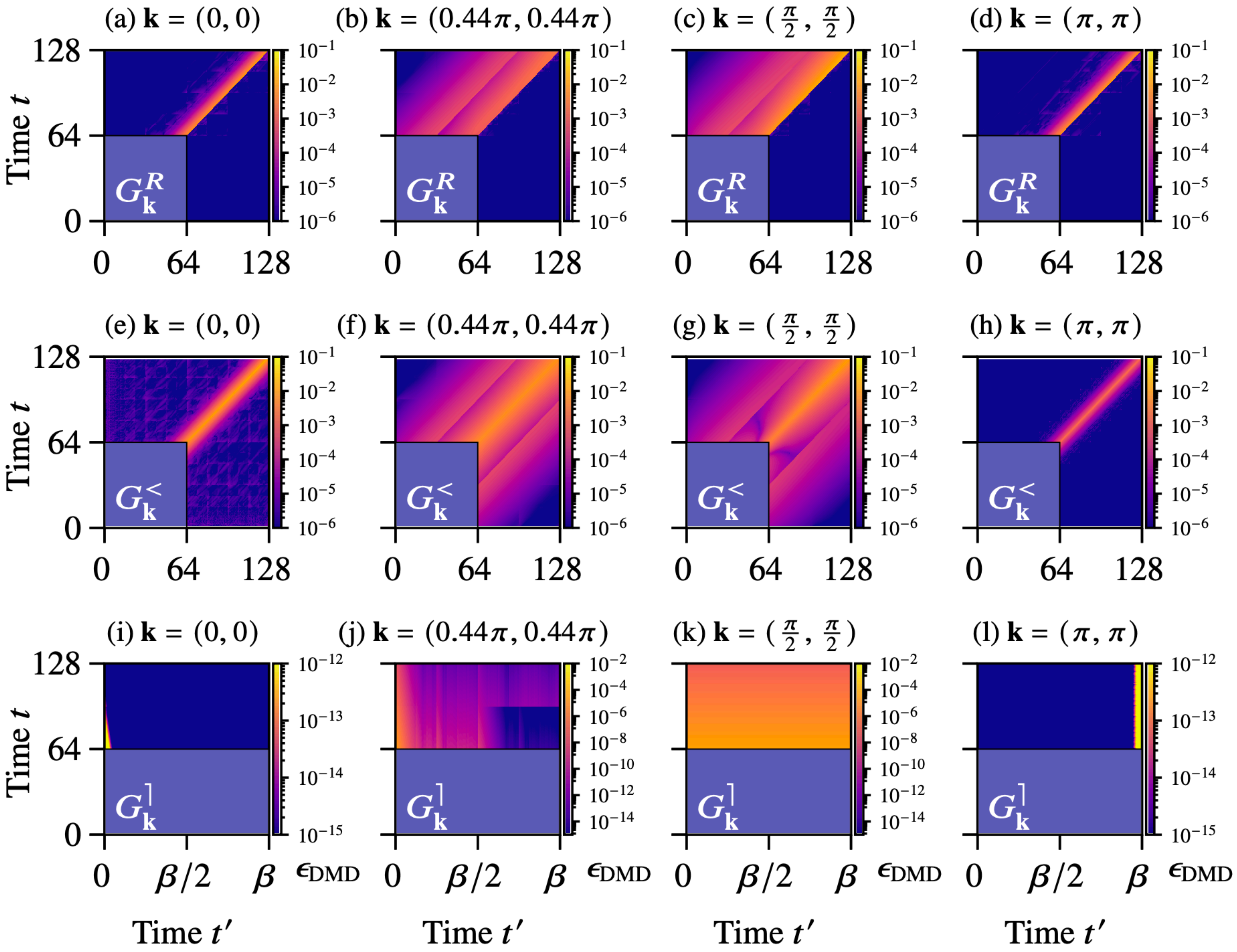
DMD guess accelerates convergence



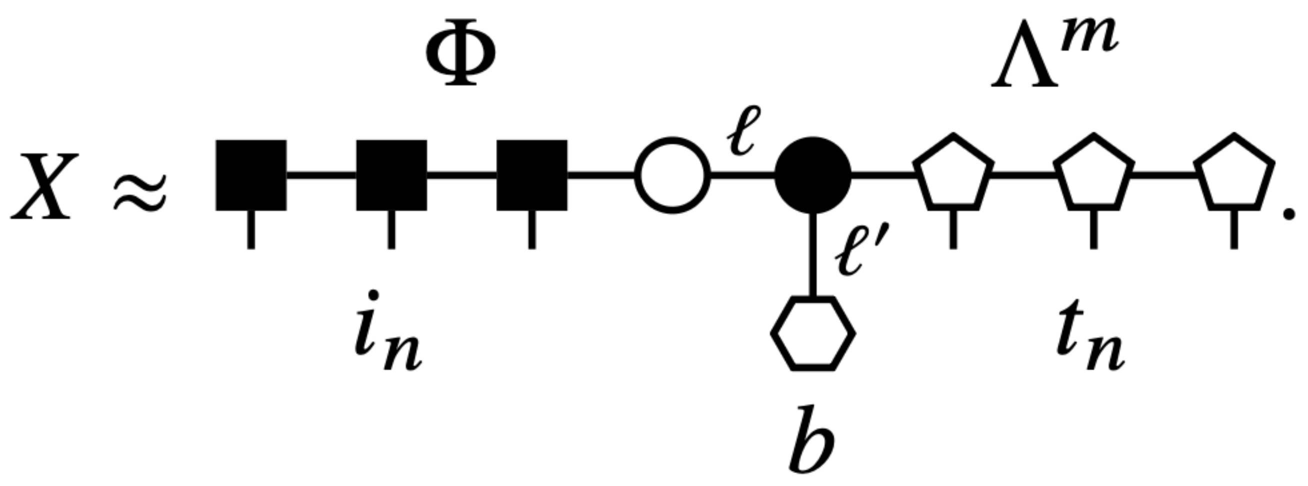
DMD guess is accurate across the BZ



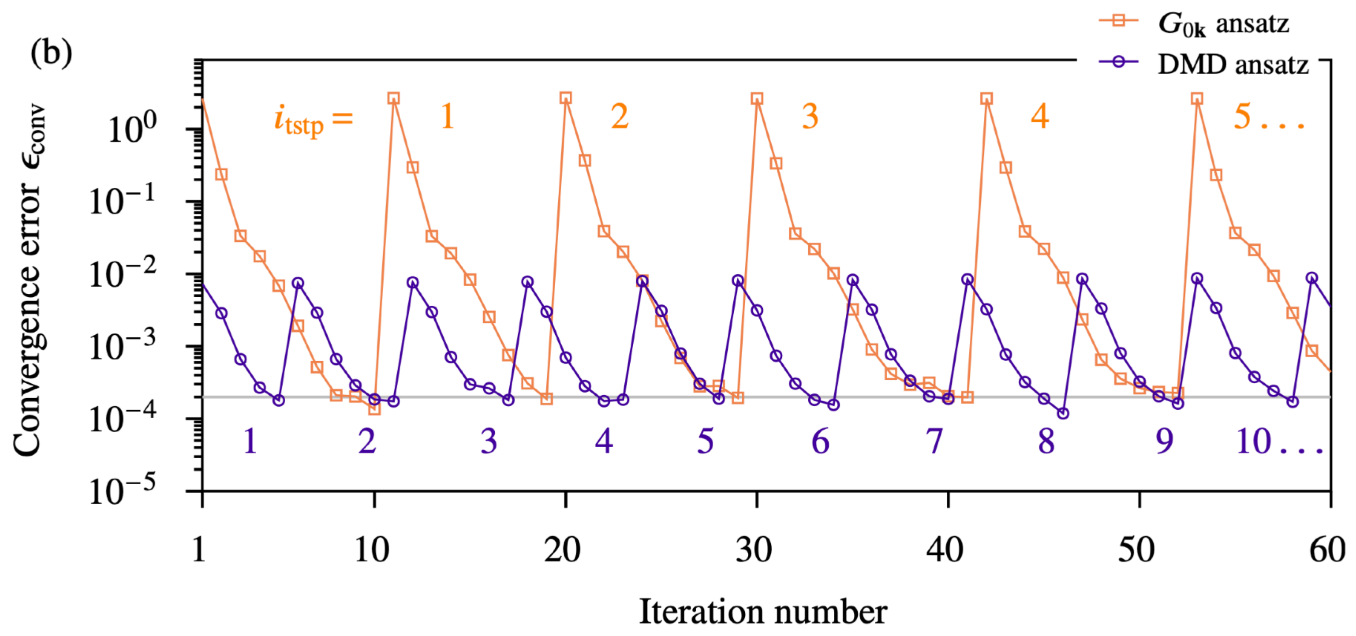
DMD guess is accurate in the two-time plane



DMD is fully composable with the QTT framework and the algorithm is straightforward



QTT-DMD provides reliable extrapolation for NEGF problems, accelerating convergence



M. Środa et al, arXiv:2509.22177, 2025

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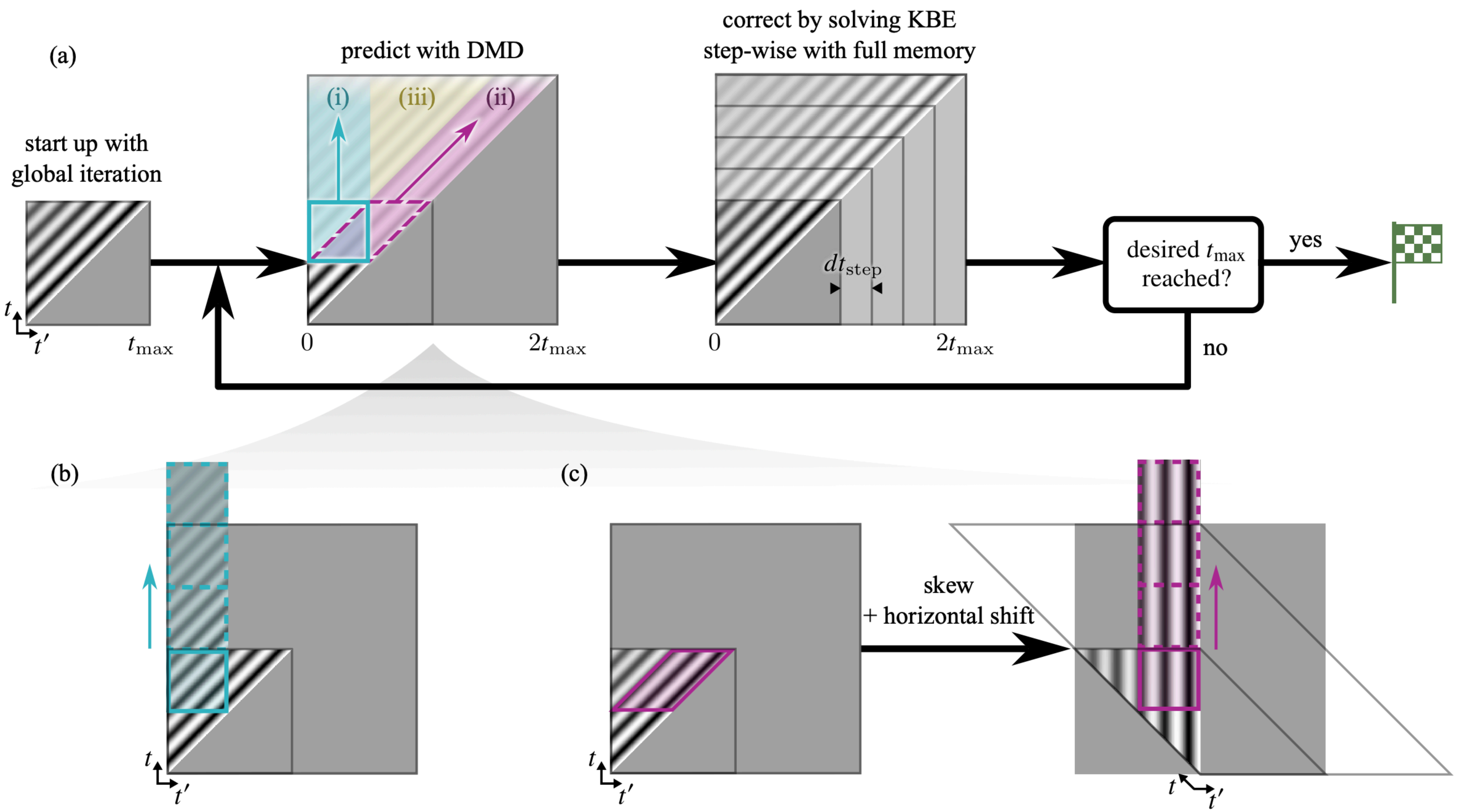
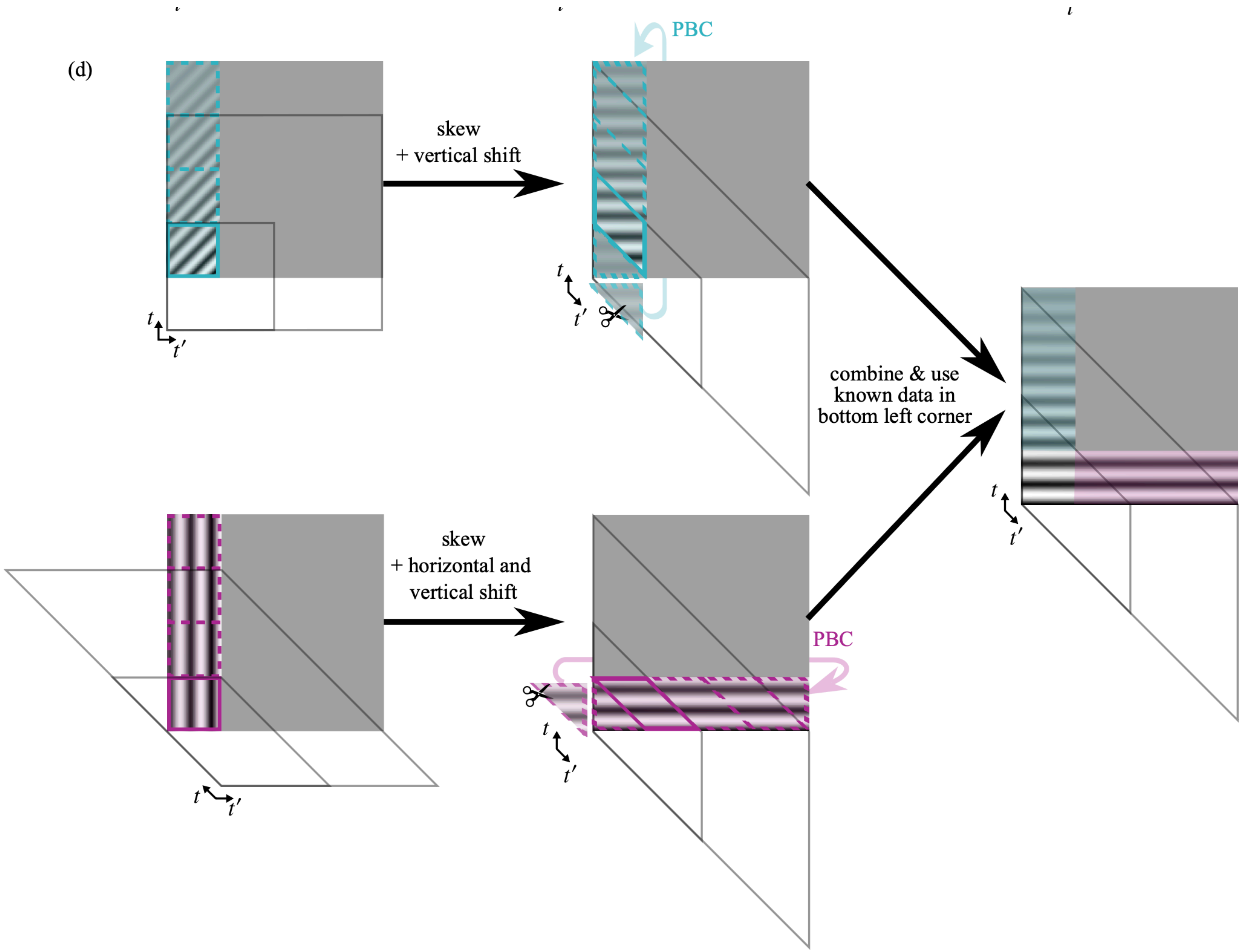
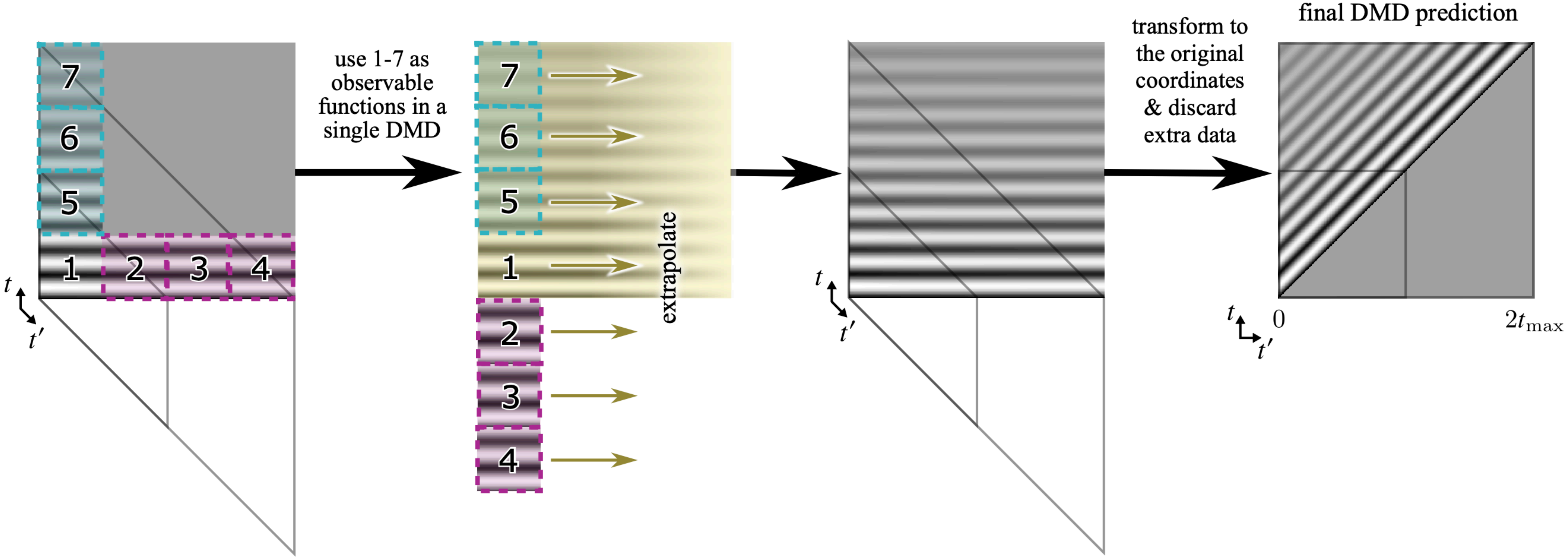


(a)
start up with
global iteration
t
t'
$t_{\max}$
predict with DMD
(i)
(iii)
(ii)
0
$2t_{\max}$
correct by solving KBE
step-wise with full memory
dt_{step}
0
$2t_{\max}$
desired $t_{\max}$ reached?
yes
no
(b)
t
t'
(c)
t
t'
skew
+ horizontal shift
t
t'


(d)
skew
+ vertical shift
PBC
t
t′
combine & use
known data in
bottom left corner
skew
+ horizontal and
vertical shift
PBC

(e)



7
6
5
1
2
3
4
t
t'
use 1-7 as observable functions in a single DMD
extrapolate
transform to the original coordinates & discard extra data
final DMD prediction
0
$2t_{\max}$