Real-time simulations on the lattice: quantum, classical and in-between

Anders Tranberg

(University of Stavanger)

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LATTICE 2024 LIVERPOOL

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Why real-time?

Many (most?) applications of lattice field theory concern the computation of correlators ***in equilibrium***, allowing Monte Carlo sampling of a Euclidean action field theory.

Very successful, Lattice 1992-2024….

Out-of-equilibrium systems are initial value problems, where some initial state evolves in real time towards a (usually unknown) final (equilibrium) state.

Lattice discretization of such systems is used in many contexts:

- Baryogenesis.
- (initial stages of) Heavy-Ion collision dynamics.
- Phase transition dynamics.
- Gravitational wave production.
- Inflation and preheating.
- Cosmic strings/monopoles/domain walls/textures…
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This talk:
- Some background for those unfamiliar with the topic.
- The problem(s).
- Solution #1: Classical-statistical.
- Solution #2: Schwinger-Dyson eqs.
- Solution #3: Going complex (briefly).
- Examples, not complete review.

Not this talk:
- AI, Quantum computing, …
- Equilibrium quantities used for real-time using linear response.
- Real-time correlators in equilibrium.
- Comprehensive review of state-of-the-art.

At Lattice 2024

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Contributions scattered over the parallel and poster sessions:

- **Eduardo Garnacho-Velasco**: In/out of eq. CME (finite T QCD).
- **Francesco d'Angelo**: QCD sphaleron rate (finite T QCD).

- **Michael Mandl, Paul Hotzy, Gert Aarts, Diaa Eddin Habibi**: Complex Langevin (algo. & AI).
- **Joshua Swaim**: Vacuum decay (algo. & AI).
- **Scott Lawrence**: Real time dynamics (algo. & AI).

- **Alexander Rothkopf**: Classical dynamics and symmetries (theor.).
- **David Weir**: Bubble nucleation (theor.).

- **Michael Hansen**: Complex Langevin Stabilization (finite density).

- **Riikka Seppä**: SU(8) bubble nucleation (poster).

- **Denes Sexty**: Real time Scalar fields (appl. outside PP).

Go check out live or poster or uploaded slides!

Introduction: Path integrals

In Quantum (Field) Theory, we often want to compute observables inside the real-time transition amplitude from one state to another:

$$\langle 2, t_2 | ... | 1, t_1 \rangle = \langle 2 | e^{-i\hat{H}(t_2 - t_1)} | 1 \rangle$$

$\hat{H}$ is the quantum Hamiltonian operator, expressed in terms of the field operators $\hat{\phi}(x,t)$.

This may be rewritten as a path integral:

$$\langle 2, t_2 | \mathcal{O}(\hat{\phi}) | 1, t_1 \rangle = \int \mathcal{D}\phi \, e^{iS[\phi]} \mathcal{O}(\phi)$$

Where S is the Lagrangian, expressed in terms of the fields, living on a time-contour in the complex plane, called $\mathbb{R}$: $[-\infty, \infty]$.

The integral is over “paths”, field configurations in 3+1 dimensions. May want to “wick rotate” to complex time, Euclidean action.

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In Thermal Quantum (Field) Theory, we often want to compute expectation values of the form:

$$\langle\mathcal{O}(\hat{\phi})\rangle = \mathrm{Tr}\hat{\rho}(t)\mathcal{O}(\hat{\phi}) = \sum_n \langle n|e^{-\hat{H}/T}\mathcal{O}(\hat{\phi})|n\rangle$$

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This may be computed order by order in perturbation theory. But not all physics is captured by such an expansion → put in on the lattice, compute it non-perturbatively.

Sometimes, one wants to actually calculate correlators with a physical time-separation:

In equilibrium:

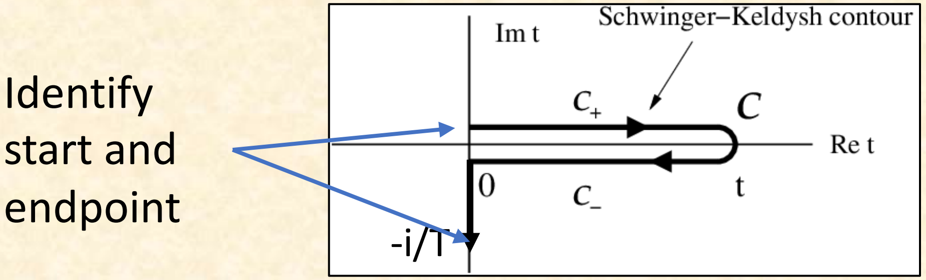
$$\langle\hat{\phi}(t_2)\hat{\phi}(t_1)\rangle = \mathrm{Tr}\hat{\rho}(t)\hat{\phi}(t_2)\hat{\phi}(t_1) =$$

$$\sum_n \langle n|e^{-\hat{H}/T}e^{-i\hat{H}(t_0-t_2)}\hat{\phi}\,e^{-i\hat{H}(t_2-t_1)}\hat{\phi}\,e^{-i\hat{H}(t_1-t_0)}|n\rangle$$

This may be rewritten as a path integral

$$\int \mathcal{D}\phi\, e^{iS[\phi]}\phi(t_2)\phi(t_1)$$

Where S is the Lagrangian, expressed in terms of the fields, living on a time-contour in the complex plane, called C, the Keldysh (or Schwinger-Keldysh) contour:



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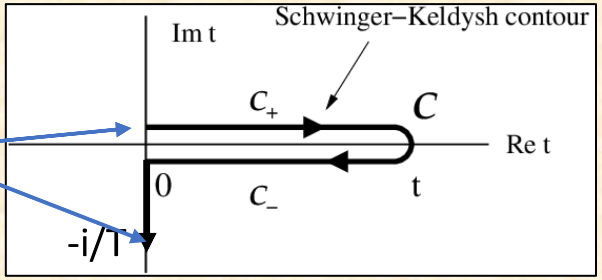
Identify start and endpoint



The initial density matrix need not be the equilibrium one. It could be any initial state.

Out of equilibrium:

$$\langle\hat{\phi}(t_2)\hat{\phi}(t_1)\rangle = \mathrm{Tr}\hat{\rho}(t)\hat{\phi}(t_2)\hat{\phi}(t_1) =$$

$$\sum_n \rho_n\langle n|e^{-i\hat{H}(t_0-t_2)}\hat{\phi}\,e^{-i\hat{H}(t_2-t_1)}\hat{\phi}\,e^{-i\hat{H}(t_1-t_0)}|n\rangle$$

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$$\int \mathcal{D}\phi\, e^{iS[\phi]}\phi(t_2)\phi(t_1)\langle\phi_0^+|\rho|\phi_0^-\rangle$$

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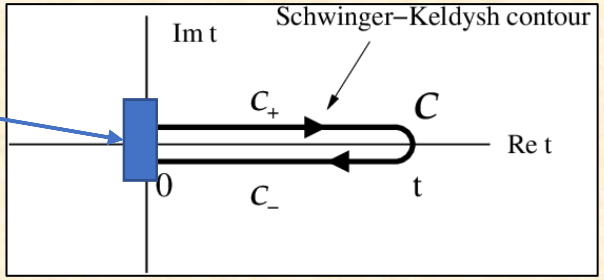
$\langle\phi_0^+|\rho|\phi_0^-\rangle$

Initial condition



The problem

But now we are in trouble!

$$P[\phi] =? \frac{e^{iS[\phi]}}{\int D\phi \, e^{iS[\phi]}}$$

Is not a probability distribution, that one may sample using importance sampling.

Alternatively, interpreting the complex phase as part of the observable,

$$\langle \mathcal{O}(\phi) \rangle =? \frac{\langle e^{iS} \mathcal{O}(\phi) \rangle}{\langle e^{iS} \rangle}$$

Converges very slowly, and the denominator is close to zero.

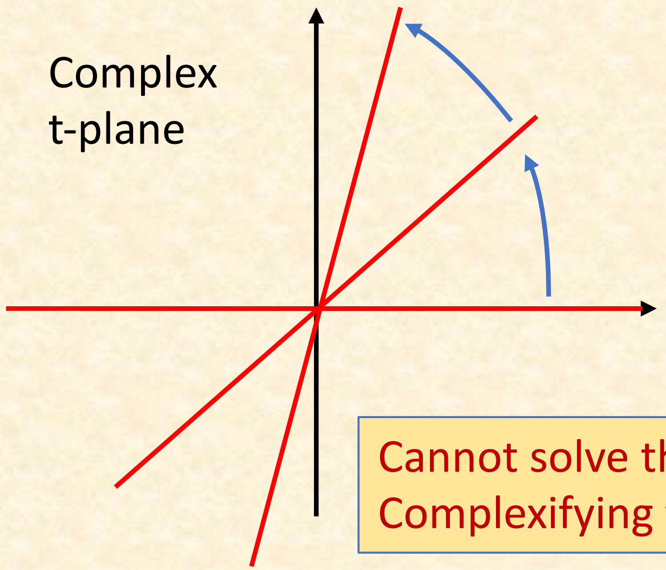
The "Sign" problem. "Exponentially hard".

Give up? Go home?

The sign problem arises whenever iS is complex, and when one cannot simply Wick rotate time t -> it and make it real:

- Equilibrium with local observables: **ok as is**!
- Vacuum-to-vacuum transitions: **ok after Wick rotation**!

- Equilibrium with time-separated observables: **Not ok**!
- Out-of-equilibrium processes: **Not ok**!
- When the system has a chemical potential
  - iS is imaginary, μN is real: **Not ok**!
  - Wick-rotate -> vice versa: **Not ok**!



Cannot solve the sign problem by Complexifying the time variable.

Solution #1: Classical-Statistical approximation

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$$\int \mathcal{D}\phi\, e^{iS[\phi]}\phi(t_2)\phi(t_1)\langle\phi_0^+|\rho|\phi_0^-\rangle$$

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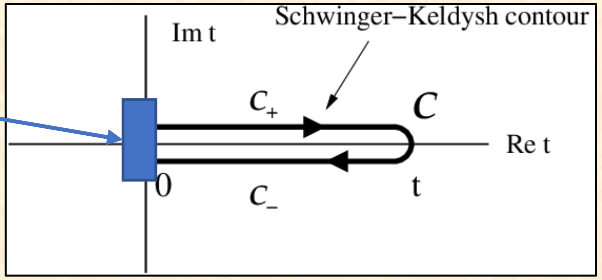

Simple statement:

- Consider only initial states ρ that are easily sample-able (like a Gaussian state). Or MC the initial state.
- Never mind sampling the inside path integral. Replace by the saddle point for each initial configuration, the classical path.

Solution #1: Classical-Statistical approximation

$$\int \mathcal{D}\phi \, e^{iS[\phi]} \phi(t_2)\phi(t_1) \langle \phi_0^+ | \rho | \phi_0^- \rangle$$

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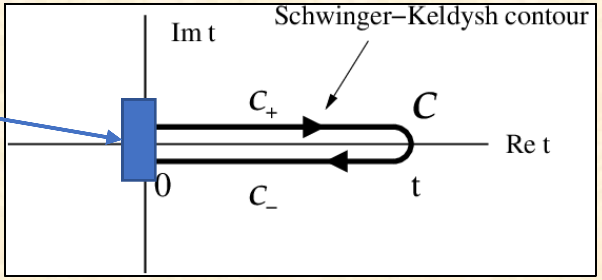
Initial condition



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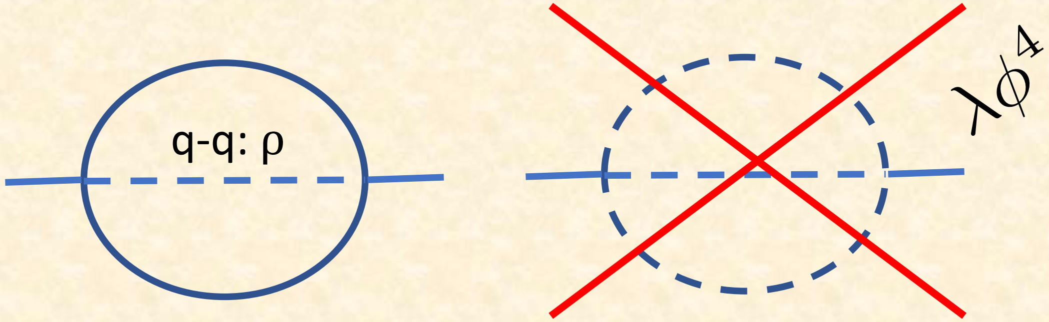
Slightly less simple statement:

- "Double" field variables by labelling with t and +/- branch.
- Redefine into Keldysh basis

$$\phi^{cl} = \frac{1}{2}\left(\phi^+ + \phi^-\right), \quad \phi^q = \phi^+ - \phi^-$$

- **Neglect all instances of $(\phi^q)^{>2}$ in the action.**
- Integrate out ϕ^q → classical eom for ϕ^{cl}.



cl-cl: F

Good approximation when

$$F^2 \gg \rho^2$$

Spectral propagator: $\rho = \langle [\phi, \phi] \rangle$ ~ 1

Statistical propagator: $F = \langle \{\phi, \phi\} \rangle$ ~ n

Aarts, Smit: 1997,
AT, Saffin, Mou, Millington: 2021

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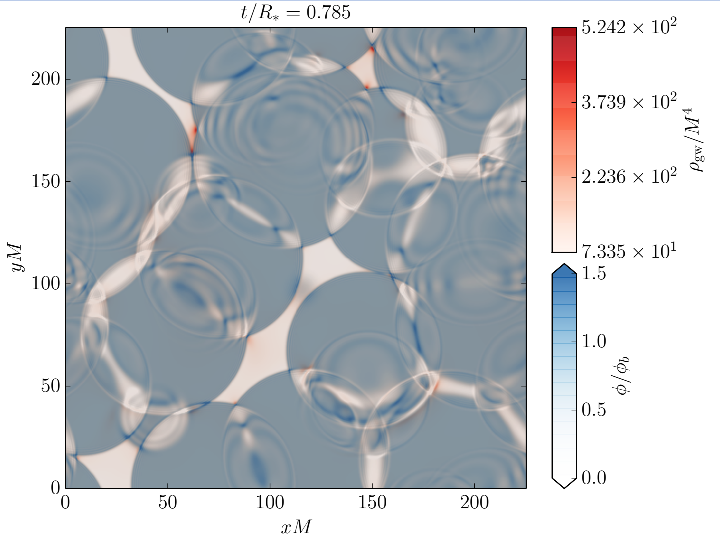
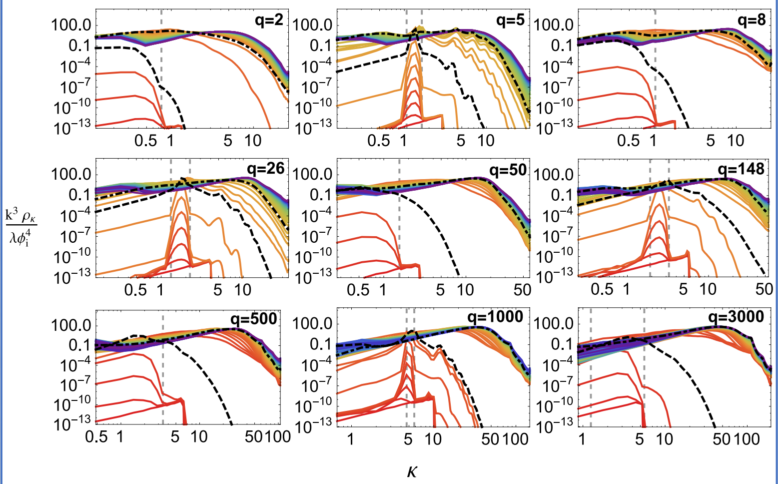
Bubbles colliding in a first order transition.
Cutting, Hindmarsh, Weir: 2018

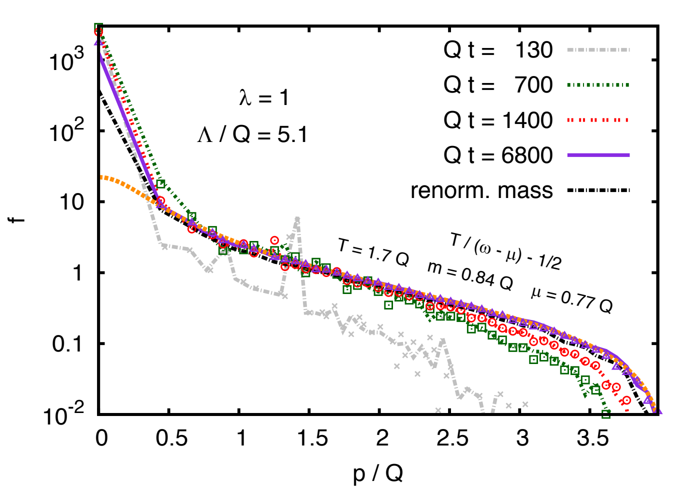


Standard lattice discretization allows for solving numerically:

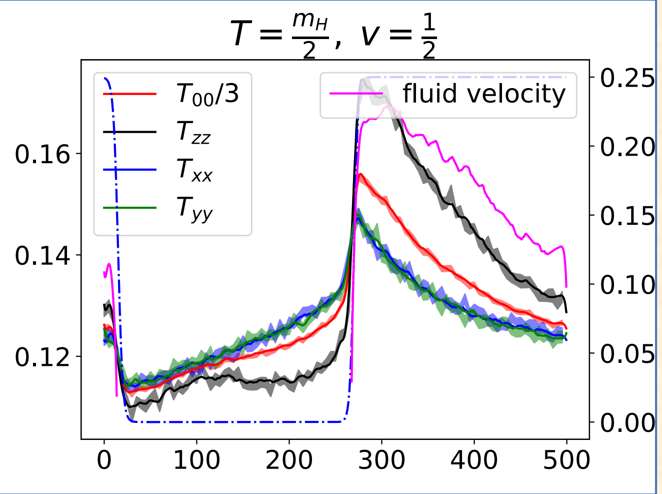
- Draw initial conditions.
- Solve equations of motion.
- Compute observables as ensemble averages.
- Make sure that volume size and resolution is sufficient.
- Numerically easy (allows for large lattices).
- Scalar fields, gauge fields, strawberry fields, …



Energy density spectra at preheating after inflation.
Figueroa, Torrenti: 2017



Occupation numbers during turbulent cascade equilibration. Berges, Boguslavski, Schlichting, Venugopalan: 2014



Energy density distribution near an advancing bubble wall.
Saffin, Mou, AT: 2020

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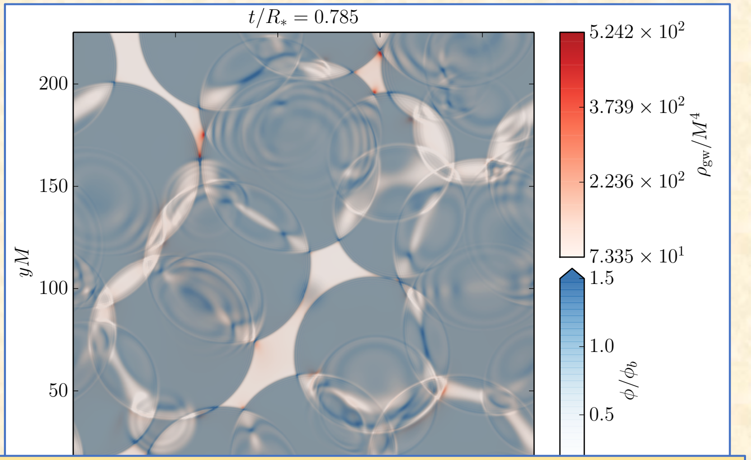

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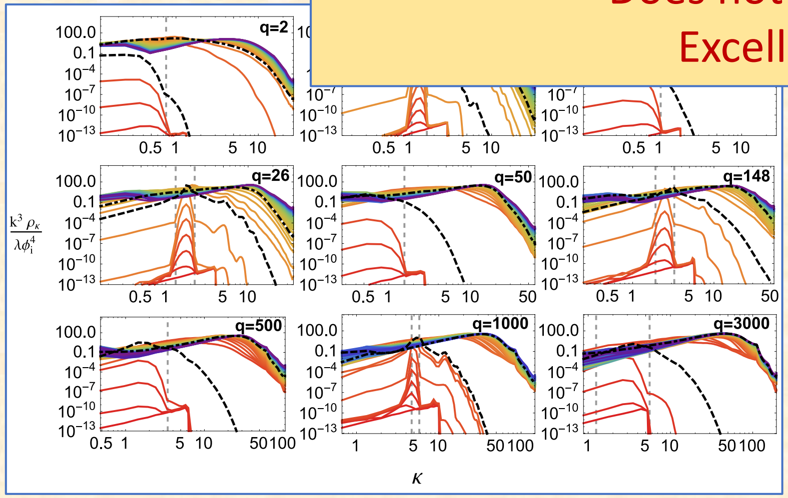
Only reliable when occupation numbers are large, F is large!
Does not give the correct equilibrium state, nor late-time behaviour.
Excellent for intermediate-time out-of-equilibrium dynamics!



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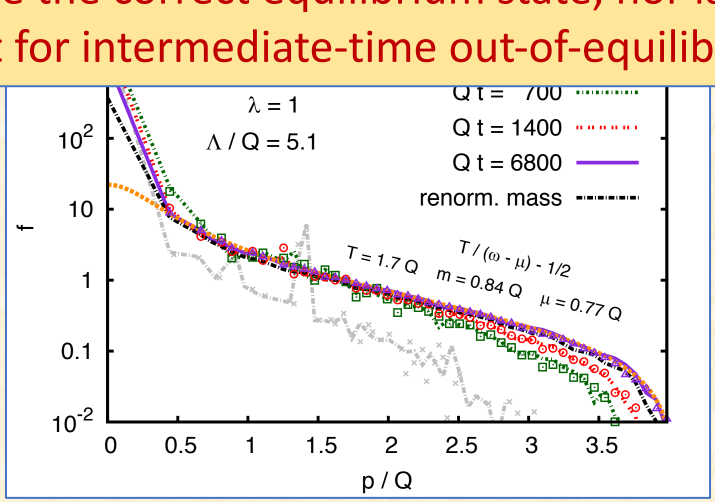

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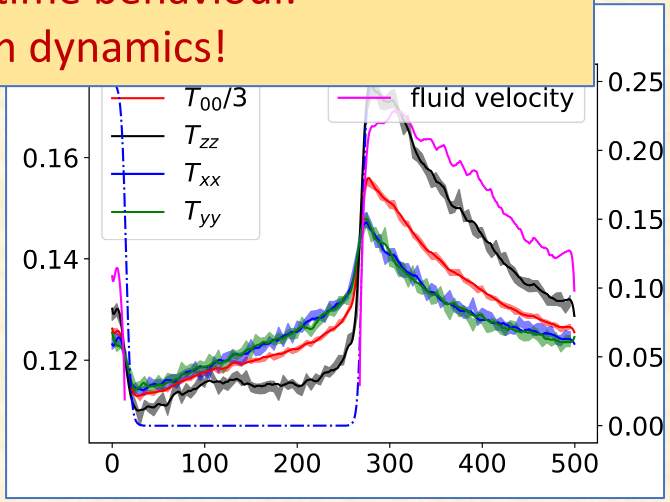

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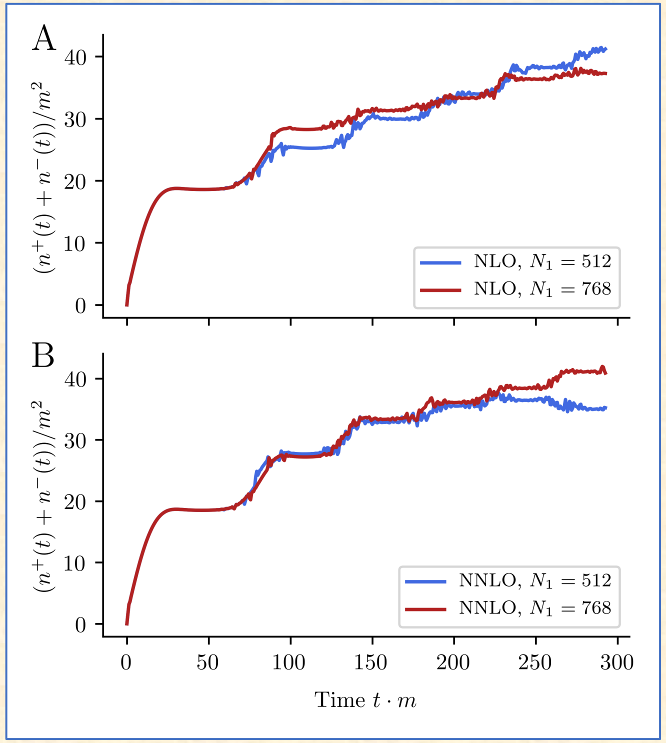
What about fermions; they do not acquire large occupation numbers?

Fermions tend to occur as bi-linears in the action → linear evolution equations. Allows for mode expansion:

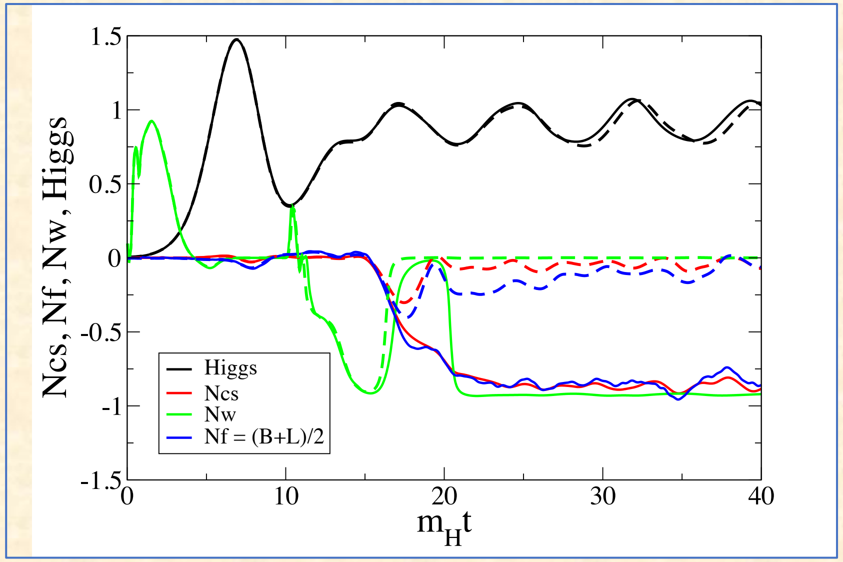
$$\psi(x,t) = \sum_{k,s} v_s a_{k,s} f_{k,s}(x,t)$$

- Solve for fermions in the classical scalar/gauge field background.
- Include back-reaction through time-dependent expectation values of fermion bilinears in classical scalar and gauge field equations of motion.

Aarts, Smit: 1998.
Hindmarsh, Borsanyi: 2009
AT, Berges, Schlichting, Mou, Saffin, …



Schwinger pair production
Spitz, Berges: 2018



Cold Baryogenesis, Nw, Ncs, Nf
AT, Saffin: 2011

Solution #2: Schwinger-Dyson equations (2PI)

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The incorrect equilibration may be ameliorated through a better treatment of the UV.

- Scale separation + effective IR dynamics with cutoff.
- Scale separation + Hard loops in UV.
- Stochastic noise/kinetic theory.

$$\left(\partial_t^2 - \partial_x^2 + M^2(x)\right)F(x,y) = -\int_0^{x^0} dz^0 \int d^3z\,\Sigma^\rho(x,z)F(z,y) + \int_0^{y^0} dz^0 \int d^3z\,\Sigma^F(x,z)\rho(z,y),$$

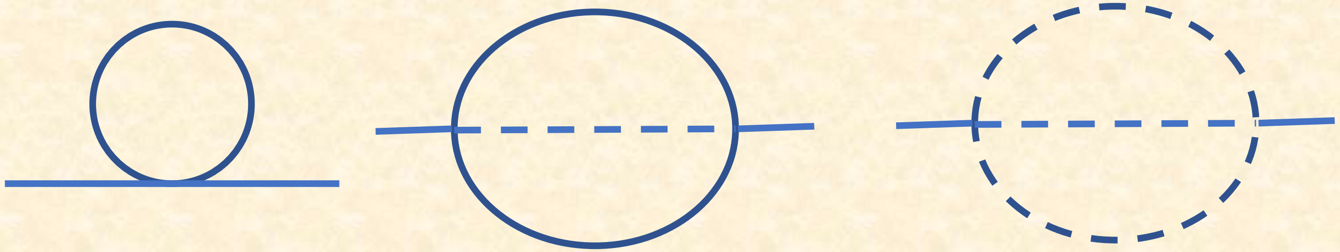
$$\left(\partial_t^2 - \partial_x^2 + M^2(x)\right)\rho(x,y) = -\int_{y^0}^{x^0} dz^0 \int d^3z\,\Sigma^\rho(x,z)\rho(z,y).$$

Statistical propagator: $F = \langle\{\phi,\phi\}\rangle$ ~ n

Spectral propagator: $\rho = \langle[\phi,\phi]\rangle$ ~ 1

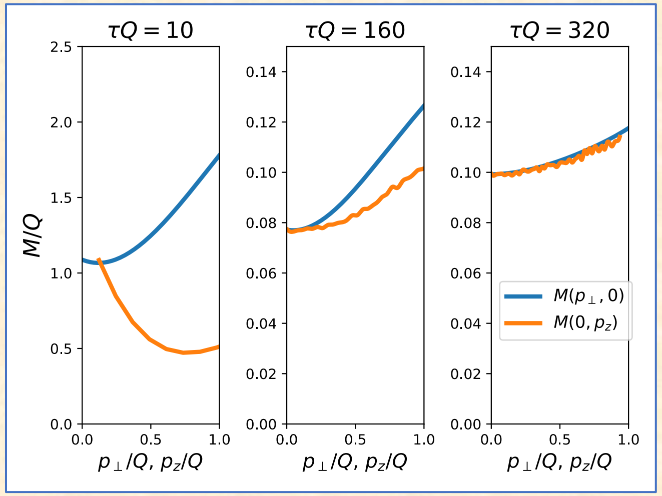
My personal favourite: Real-time Schwinger-Dyson equation based on truncation of 2PI effective action.

- Provides self-consistent evolution equations for full correlation functions.
- Beyond LO, involves memory integrals to the initial time.
- Conveniently discretized through a lattice action (or ad hoc).
- Conserves energy, Goldstone theorem, Ward identities, renormalisability.
- Thermalises to quantum equilibrium.
- Reliable also for small occupation numbers.
- Systematically improvable.

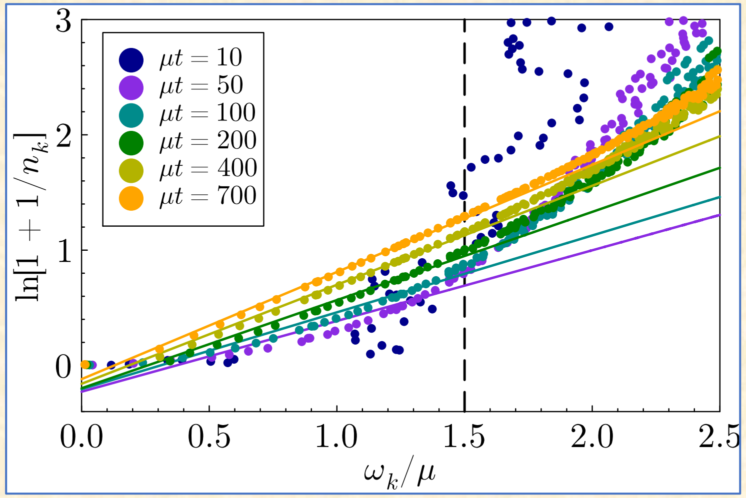


Berges, Cox: 2001
Aarts, Berges: 2002, …
Aarts, Berges, Serreau, Baier, Ahrensmeier: 2002
AT, Smit, Arrizabalaga: 2004 + 2005.
AT: 2008

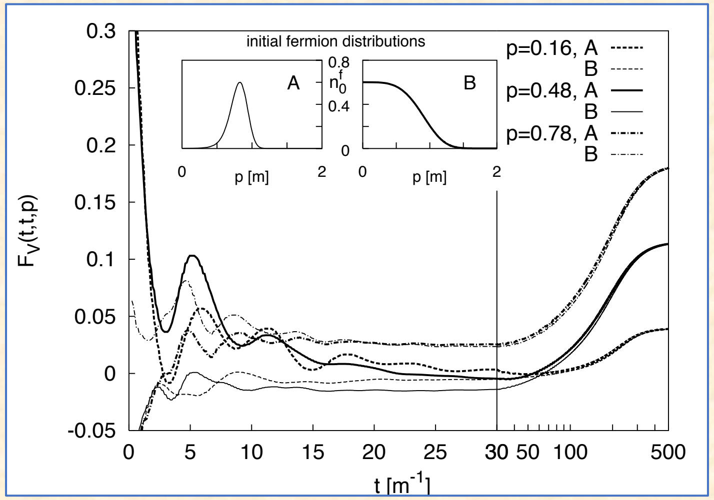
- Numerically hard (time and memory intensive).
- Scalars and fermions ok (doublers, …).
- Gauge fields much harder.
- Hard to go beyond NLO.
- Renormalisation works, but hard.
- Resummed perturbative. Unlikely to capture truly non-perturbative properties (defects, instantons, confinement?)



Thermal mass in expanding (scalar field) plasma
Gelis, Hauksson: 2024



Thermalisation after preheating
Ungersbäck, AT: 2024



Fermion thermalisation
Berges, Borsanyi, Serreau: 2003

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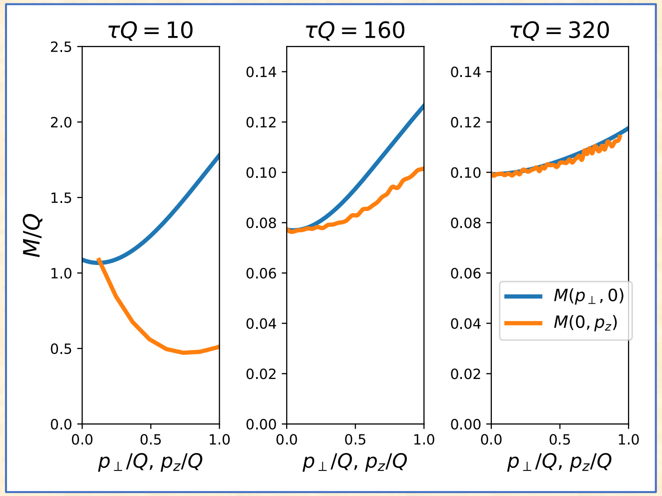
- Use, when classical-statistical approximation fails.



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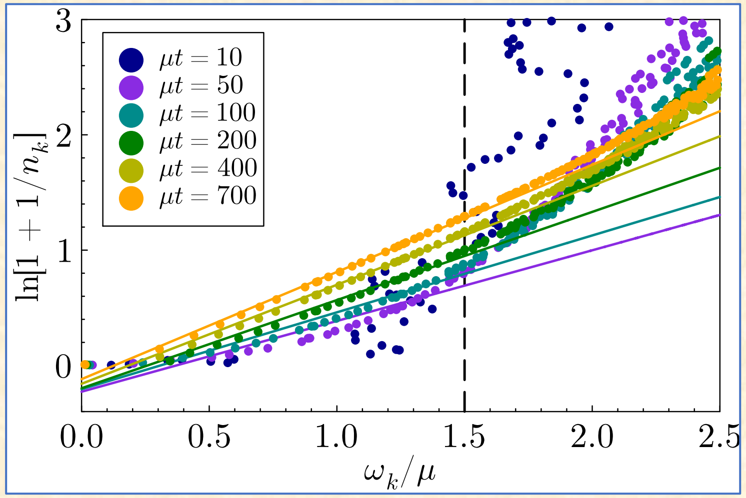

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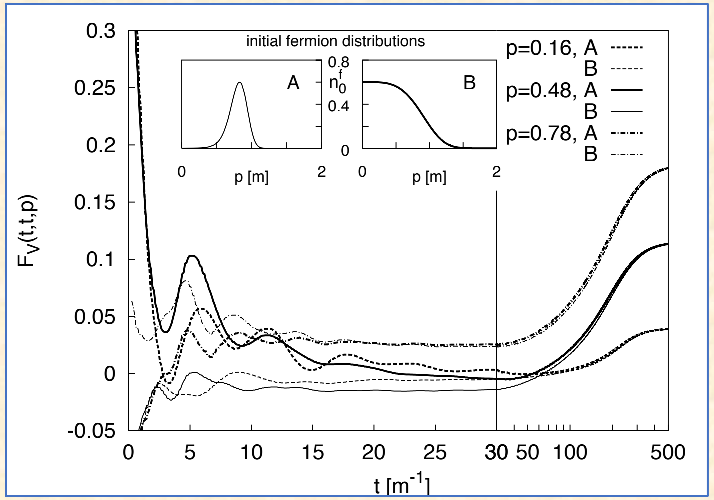

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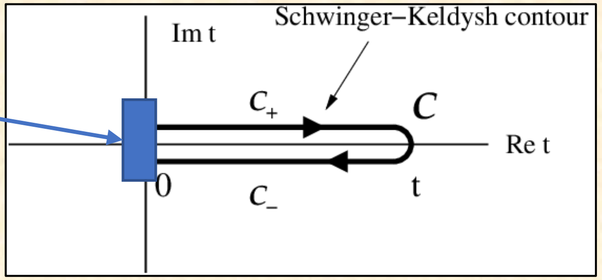
Solution #3: Going complex

Contour deformation (Thimbles)

$$\int \mathcal{D}\phi \, e^{iS[\phi]} \phi(t_2)\phi(t_1)\langle\phi_0^+|\rho|\phi_0^-\rangle$$

$\langle\phi_0^+|\rho|\phi_0^-\rangle$

Initial condition



To get full nonperturbative quantum results, must evaluate entire path integral.

Bad convergence when field variables are on the (real axis)^N. Find a better "axis"? Not complex time path; complex-valued field variables, allowed to probe hypersurface in in C^N.

- Continuous deformation from R^N (Generalised Thimble).
- Directly on "optimal" manifolds (Lefschetz Thimbles).
- Maths tells you the result is the same. Is the numerical effort sufficiently reduced?

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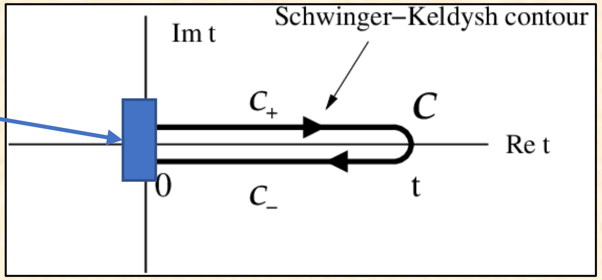

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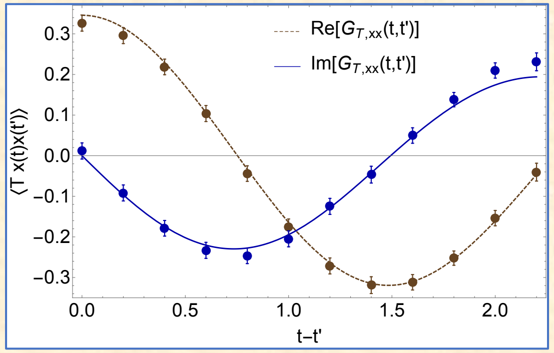
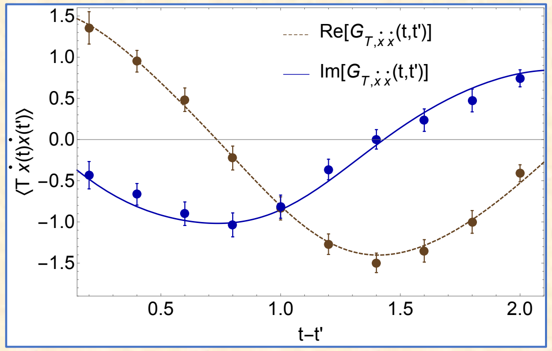
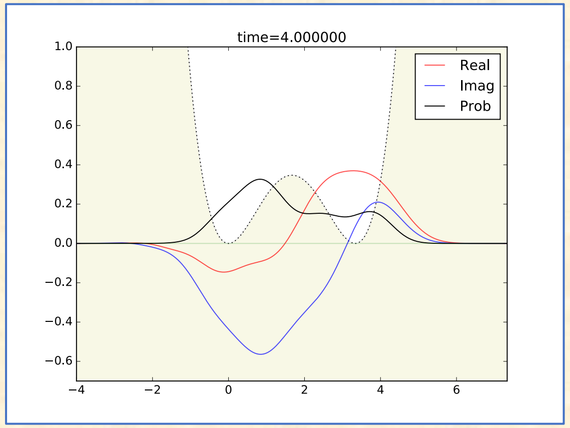
Sofar, only very short physical times are accessible.

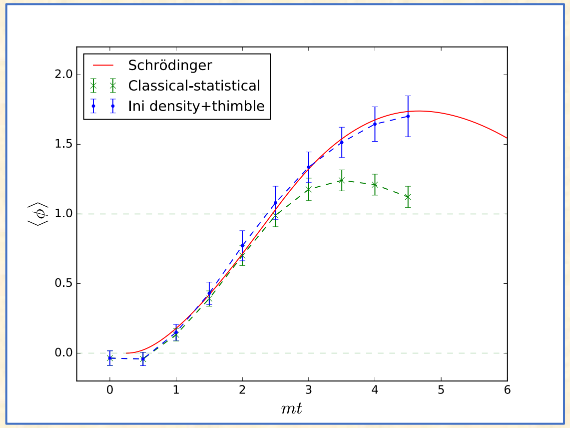




Correlators in QM. Also 1+1d field theory from same group.
Alexandru, Basar, Bedaque, Vartak, Warrington: 2016

Quantum mechanical tunneling
AT, Mou, Saffin: 2019



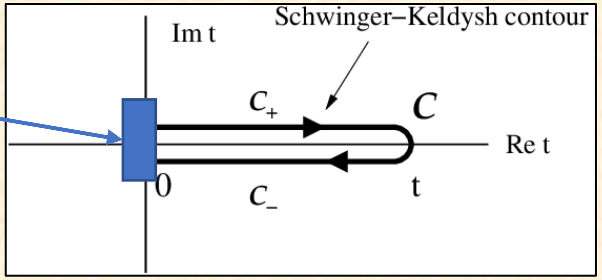


Complex Langevin

$$\int \mathcal{D}\phi \, e^{iS[\phi]} \phi(t_2)\phi(t_1)\langle \phi_0^+|\rho|\phi_0^-\rangle$$

$\langle \phi_0^+|\rho|\phi_0^-\rangle$

Initial condition



To get full nonperturbative quantum results, must evaluate entire path integral.

For a Euclidean action/positive definite distribution, sample using MC or Langevin/stochastic quantization.

For a complex action → do the same! It might just work.
Not complex time path; complex-valued field variables, each allowed to probe all of the complex plane.

Issues of convergence and stability can be tempered through field redefinitions/kernels, dynamical stabilization. Much harder for real-time evolution than for chemical potential.

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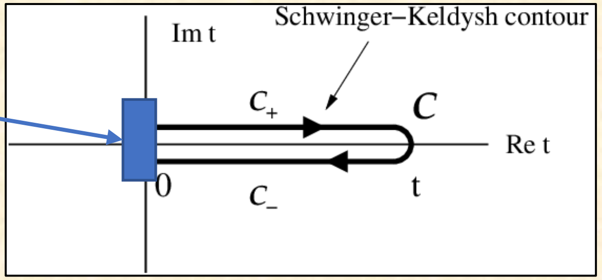

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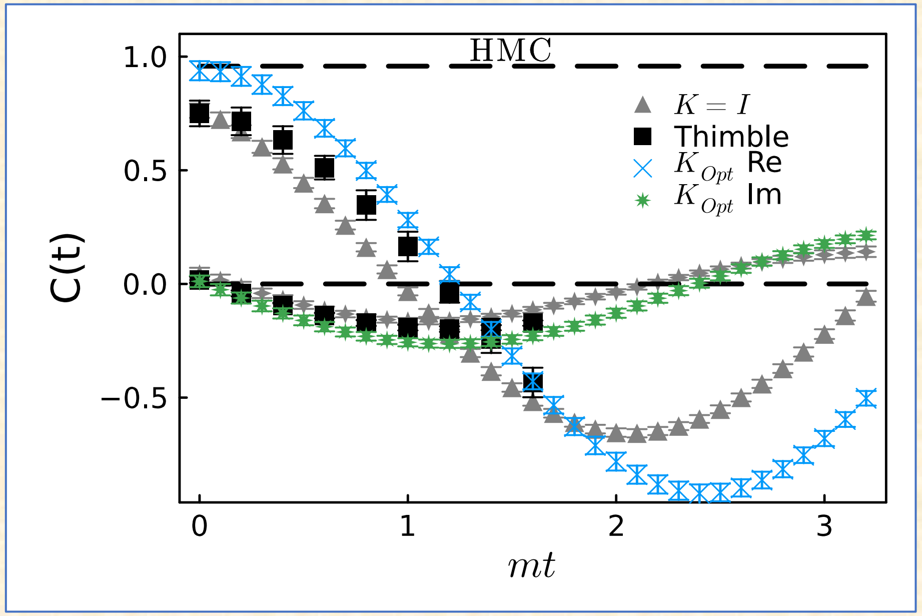
1+1 d, non-equal-time correlator. ML, kernels, …
Sexty, Alvestad, Rothkopf: 2024 (talk Tuesday)



Conclusion and outlook

University of Stavanger

- Lattice quantum field theory methods are used to study many out-of-equilibrium phenomena in cosmology, early Universe phase transition physics and heavy ion collisions.

- Initial value problems in real time suffer from a severe sign problem, and computing the path integral is mostly replaced by:
  - Classical-statistical simulations (when that applies), sometimes with quantum fermions.
  - UV-improved, perturbatively embellished evolution equations (when they work).

- Focus has been to reach large volumes with fine resolution, large physical times, expanding boxes, many different models, several mass scales. Much phenomenological exploration, but also numbers (or exponents, space/time scales, spectra) matched to experiment and observation.

- For truly non-perturbative, but also truly quantum, real-time evolution, we await that Complex Langevin and/or Thimble simulations extend to long times and large volumes in 3+1D.

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Thank you for your attention!