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

Anders Tranberg[a,*]

[a] *Faculty of Science and Technology, University of Stavanger, 4036 Stavanger, Norway*

E-mail: anders.tranberg@uis.no

I give a brief introduction to the use of lattice field methods for studying quantum evolution (way) out of equilibrium. I emphasize the way in which the numerically simple, and very successful, classical-statistical approximation is related to the much more involved quantum evolution and the 2PI-formalism which in a sense is in-between. I give some illustrative examples of seminal and recent applications of these methods. This is not meant as a comprehensive and balanced review of the state-of-the art of the field, but as a primer and overview for lattice field theory scientists interested in making an excursion from 4-D Euclidean space to 3+1 Minkowski signature.

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1. Introduction: Why real-time?

Lattice field theory was orignally designed to provide a robust regularization of quantum field theory (QFT), explicitly preserving gauge symmetry. In the early 80's, nonperturbative numerical investigations of QFT (QCD) were centered on computing path integrals through importance sampling. In Euclidean space (either for vacuum transitions through Wick rotation or in thermal field theory), the integrand of the path integral is indeed positive definite and suitable as a probablity distribution.

However, many interesting phenomena in physics are out of thermal equilibrium and present evolution in real-time from some initial condition to an apriori unknown final state. Examples pertinent to the patrons of the Lattice conference series include phase transition dynamics, the initial stages of heavy-ion collisions, bubble nucleation, baryogenesis, inflation, reheating, and topological defects such a monopoles, cosmic strings and domain walls. For those phenomena, the path integral can no longer be (efficiently) sampled statistically, as the integrand is manifestly a complex phase. On the other hand, Lattice regularization still provides a convenient tool for making the problem numerically tractable.

In order to set the stage, I will first make some general remarks on the path integral in real-time, emphasizing why this is different from standard equilibrium Lattice QFT. I will then proceed to introduce three avenues to computing the real-time out-of-equilibrium evolution quantum systems, and provide some examples from the literature. These are the Classical-Statistical approximation (CS), the Real-time Schwinger-Dyson (Kadanoff-Baym, 2PI) equations and direct evaluation of the path integral through complexification of the field variables (Complex Langevin and Picard-Lefshetz thimbles). I end with a brief summary.

2. Path integrals and a problem

Path integrals in Euclidean time

In QFT, we often seek to compute expectation values of observables inside the real-time transition amplitude from one state to another:

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

where $\hat{H}$ is the quantum Hamiltonian operator generating time evolution, expressed in terms of some field operators $\hat{\phi}(x,t)$. This may be rewritten as path integral:

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

where S is the action, expressed in the (number-valued) field variables ϕ, that live on a particular time contour in the complex plane called $\mathbb{R}:[-\infty,\infty]$. $\mathcal{D}\phi$ denotes that there is one integration variable for each point in 3+1 dimensional space time, x,t. It is often convenient to Wick rotate the time coordinate into the complex plane, to get a Euclidean space-time and a Euclidean action allowing for importance sampling.

In Thermal QFT, we similarly often want to compute expectation values of the form:

$$\langle O(\hat{\phi})\rangle = \mathrm{Tr}\hat{\rho}(t)(O)\hat{\phi} = \sum_n \langle n|e^{-\hat{H}/T}O(\hat{\phi})|n\rangle. \tag{3}$$

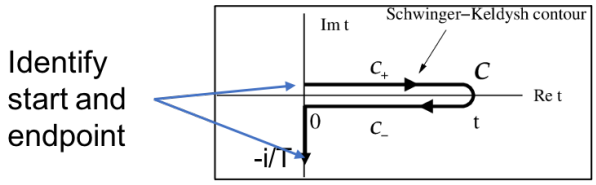

Figure 1: Field variables live on a time contour in the complex plane. In thermal equilibrium, field variables are enforced to be periodic, and the contour extended to $-i/T$.

In this context the Hamiltonian $\hat{H}$ is not there to generate time evolution, but enters in the density matrix in thermal equilibrium. Still, since the Hamiltonian is the Hamiltonian, this may also be written as path integral:

$$\langle O(\hat{\phi})\rangle = \int \mathcal{D}\phi e^{-S_E[\phi]} O(\phi), \tag{4}$$

where S_E is the Euclidean action, expressed in terms of the (number-valued) field variables ϕ, that lie on a particular time-contour in the complex plane $[0.-i/T]$. As before, $\mathcal{D}\phi$ denotes integrating over field variables, one for each x,τ in this 4 dimensional space, but now with the constraint that the fields are periodic in the time direction.

Either of these computations can be done analytically order by order in continuum perturbation theory, in lattice discretized perturbation theory, or non-perturbatively on the lattice by (numerical) importance sampling. Then $\mathcal{D}\phi$ denotes a finite number of integration variables, corresponding to a discrete set of x,t (or τ).

Path integrals in real time

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

$$\langle\hat{\phi}(t_2)\hat{\phi}(t_1)\rangle = \mathrm{Tr}\hat{\rho}(t)\hat{\phi}(t_2)\hat{\phi}(t_1) = \sum_n \langle n|e^{-\hat{H}/T}e^{-i\hat{H}(t_0-t_2)}\hat{\phi}e^{-i\hat{H}(t_2-t_1)}\hat{\phi}e^{-i\hat{H}(t_1-t_0)}|n\rangle. \tag{5}$$

This may be rewritten as a path integral

$$\int \mathcal{D}\phi e^{iS[\phi]}\phi(t_2)\phi(t_1), \tag{6}$$

where S is the action, expressed in terms of field variables living on a particular time-contour in the complex plane, the Keldysh (or Schwinger-Keldysh) contour C (see Fig. 1). These field variables are often denoted with a physical time label and ϕ^+, ϕ^-, depending on whether they are on the upper (C_+) or lower (C_-) branch.

But the initial density matrix need not be the equilibrium one. It could be any initial state, such that the subsequent evolution is out of equilibrium:

$$\langle\hat{\phi}(t_2)\hat{\phi}(t_1)\rangle = \mathrm{Tr}\hat{\rho}(t)\hat{\phi}(t_2)\hat{\phi}(t_1) = \sum_{mn}\rho_{mn}\langle n|e^{-i\hat{H}(t_0-t_2)}\hat{\phi}e^{-i\hat{H}(t_2-t_1)}\hat{\phi}e^{-i\hat{H}(t_1-t_0)}|m\rangle. \tag{7}$$

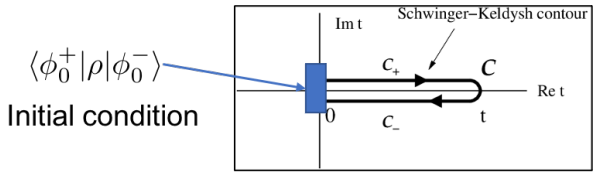

Figure 2: Field variables live on a time contour in the complex plane. Out of equilibrium, the end points are related by an initial density matrix, to be specified.

This may be rewritten as a path integral

$$\int \mathcal{D}\phi e^{iS[\phi]}\phi(t_2)\phi(t_1)\langle\phi_0^+|\rho|\phi_0^-\rangle = \int \mathcal{D}\phi_0^{+/-}\langle\phi_0^+|\rho|\phi_0^-\rangle \int \mathcal{D}\phi_{\neq 0}^{+/-} e^{iS[\phi]}\phi(t_2)\phi(t_1), \tag{8}$$

where S is the action, expressed in term of fields variables ϕ^+, ϕ^-, living on a particular time contour in the complex plane similar to the previous one (also known as the Keldysh contour), but without the branch to $-i/T$ (see Fig. 2). The end point field configurations ϕ_0^+, ϕ_0^- are no longer identified for periodicity, but are related through the matrix element $\langle\phi_0^+|\rho|\phi_0^-\rangle$. For later use, we have also written a version where the initial conditions are part of a separate outer integral.

A problem

But now we are in trouble. The object

$$P[\phi] = ? \frac{e^{iS[\phi]}}{\int \mathcal{D}\phi e^{iS[\phi]}}, \tag{9}$$

is not a positive definite function of the fields, and cannot be used as a probability distribution for importance sampling. Alternatively identifying the complex phase as an observable

$$\langle O(\phi)\rangle ? = \frac{\langle e^{iS} O(\phi)\rangle}{\langle e^{iS}\rangle}, \tag{10}$$

also does not work, since it is an oscillating function for which the integral converges extremely slowly. This is a "sign" problem, a challenge for non-zero chemical potential (where one may Wick rotate most of the action to Euclidean signature), and even worse for real-time evolution (where Wick rotation is not an option). It appears that one cannot solve the sign problem by complexifying the time, t.

3. Solution #1: The classical-statistical approximation

The most popular solution to the problem is to note that many out-of-equilibrium phenomena involve large occupation numbers, at least in the physcially most relevant parts of the spectrum. Typical examples are topological defects, which are large-amplitude fields, or instabilities and resonances, where some modes grow to be very large. The simple prescription is then to replace the quantum evolution by classical equations of motion, and the initial state density matrix by an ensemble of statistically independent realisations. This is known as the classical-statistical approximation (CS).

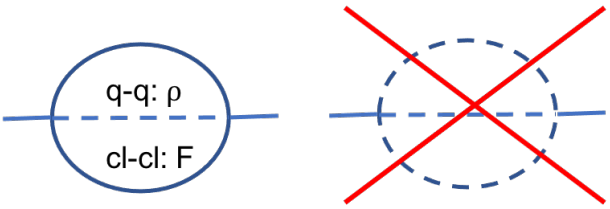

Figure 3: NLO diagrams with $3 \times cl + 1 \times q$ vertices (left) that are "classical" and $1 \times cl + 3 \times q$ vertices (right) that are "quantum", and neglected in CS.

Numerically, it amounts to drawing a suitable number of random lattice discretized configurations from the initial state ensemble, and evolving them using the equations of motion. Subsequently one may compute whatever classical observable one chooses at any later time, by averaging over the set of configurations. This prescription is very simple, numerically efficient and allows for fairly high accuracy and/or very large lattices in three spatial dimensions.

Why CS is sensible to do

CS is not simply an ad-hoc prescription, but a well defined approximation [1], which can be made more concrete than the "large occupation numbers" criterion. Consider the path integral on the Keldysh contour, and redefine the field variables

$$\phi^{cl} = \frac{1}{2}\left(\phi^{+} + \phi^{-}\right), \quad \phi^{q} = \phi^{+} - \phi^{-}. \tag{11}$$

These are often referred to as "classical" and "quantum" fields, respectively. Now imagine that one had a standard ϕ^4 scalar theory, then the lagrangian would include interactions of the form (the minus sign follows from going forwards and backwards in C_+, C_-)

$$\lambda(\phi^{+})^4 - \lambda(\phi^{-})^4 = 32\phi_{cl}^3\phi_q + 8\phi_{cl}\phi_q^3, \tag{12}$$

There are vertices of the type $(\phi^{cl})^3\phi^q$ and the type $(\phi^q)^3\phi^{cl}$, generating diagrams of the form show in Fig. 3. Full lines are $\phi^{cl} - \phi^{cl}$ propagators (statistical correlators F), while dashed lines are $\phi^q - \phi^q$ propagators (spectral correlators ρ). Hence these two diagrams are of the form $F^2\rho + \rho^2\rho$ (up to signs and combinatorial factors). Note that external lines are always ϕ^{cl}. The classical approximation amounts to neglecting the $(\phi^q)^3\phi^{cl}$ vertex, or equivalently the ρ^3-diagram.

One may always apply this approximation, but it is only a *good* approximation when $F^2 \gg \rho^2$. It is not hard to convince oneself, that for small coupling (in the quasiparticle range), in momentum space:

$$F(k) \propto \frac{n_k + 1/2}{\omega_k}, \qquad \rho(k) \propto \frac{1}{\omega_k}, \tag{13}$$

where n_k is the occupation number of mode k, in which case the criterion $F^2 \gg \rho^2$ reduces to "large occupation numbers",

$$n_k \gg 1. \tag{14}$$

The CS approximation may also be understood in terms of (8), by noting that it amounts to performing the outer integral over initial conditions, but replacing the inner integral by a saddle point approximation keeping $\phi_0^{\pm}$ fixed [2].

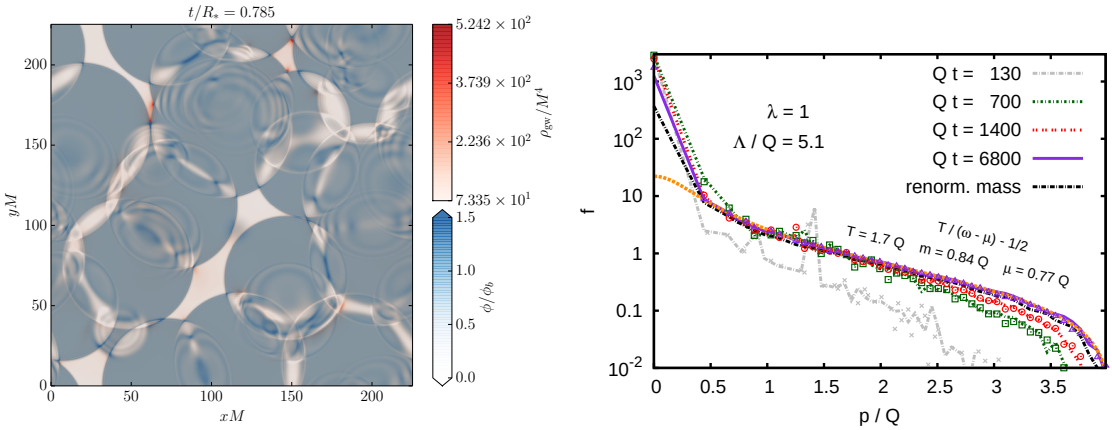

Figure 4: Left: Snapshot of a bubble nucleation simulation, as the bubbles begin to coalesce. (Reproduced from [3] with kind permission from the authors). Right: Time evolution of spectra of occupation numbers during turbulent thermalisation. (Reproduced from [5] with kind permission from the authors).

What CS is useful for

The CS approximation has been applied to a host of phenomena in high-energy physics and early Universe cosmology. Examples include:

- Bubble nucleation dynamics in first order phase transitions, Fig. 4 (left, [3]). The figure shows a slice through a lattice full of nucleated bubbles. At this time, several bubbles have nucleated and started to collide and coalesce. As a further application, one may compute the energy-momentum tensor, and demonstrate that bubble collisions and subsequent plasma dynamics generates gravitational waves, potentially observable with the LISA detector [4].

- Equilibration dynamics in heavy-ion collisions, Fig. 4 (right, [5]). The figure shows the particle spectrum at early, late and intermediate times during a stage of turbulent equilibration for a scalar field plasma.

- Reheating dynamics of scalar (and gauge) fields after inflation, Fig. 5, [6]. The figure shows the energy density spectra during resonant preheating for different times (lines of different colour) for different values of a characteristic resonance parameter q. Modes in a resonance band with the inflaton field (near $k = 1, ..., 5$) are amplified. Again, the ultimate goal is to compute the gravitational wave signal from such a preheating period in the early Universe.

- Out-of-equilibrium dynamics of an advancing bubble wall interacting with a gauge-scalar plasma, Fig.6, [7]. The figure shows the diagonal components of the energy-momentum tensor of the plasma along the direction perpendicular to the advancing wall.

3.1 What CS cannot do

The CS approximation is not a silver bullet enabling computation of any quantum evolution, and has a number of shortcomings:

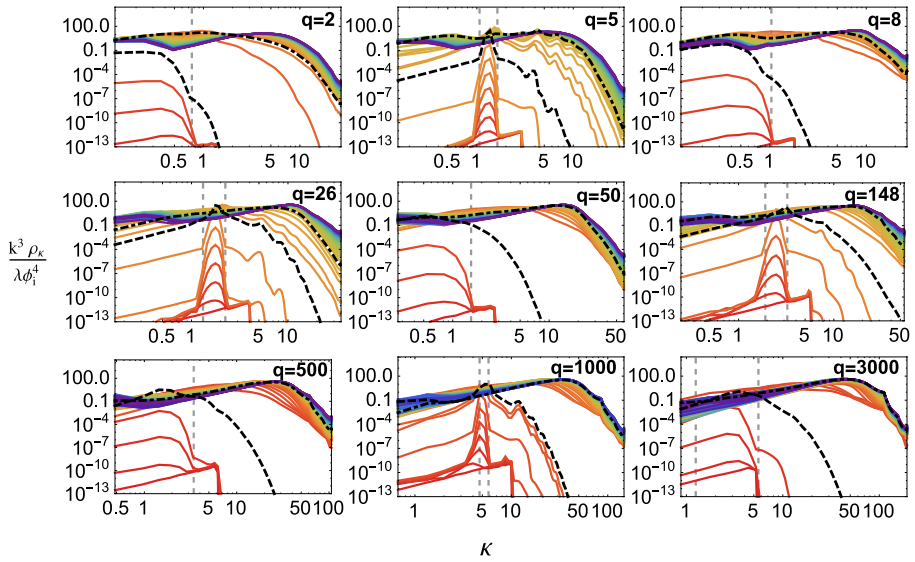

Figure 5: Time evolution of spectra of the energy density in resonant preheating for different instances of the resonance parameter q. (Reproduced from [6] with kind permission from the authors).

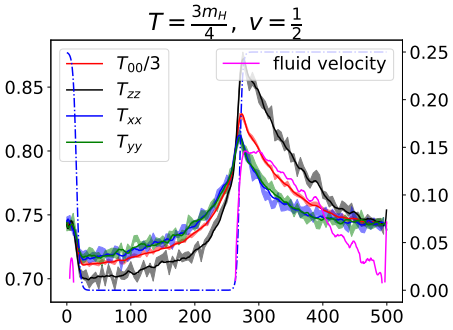

Figure 6: Energy density components of an electroweak plasma near an advancing bubble wall. (Reproduced from [7] with kind permission from the authors).

- It does not work very well for small occupation numbers. Quantum phenomena that do not involve large-amplitude fields are not well approximated
- CS thermalises to the classical vacuum rather than the quantum one. In particular, the far UV modes (where occupation numbers are small) equilibrate to the wrong state, resulting in the usual Rayleigh-Jeans problem. On a lattice, the temperature becomes cut-off dependent.
- Some works involving CS simulations have been initialised with an ensemble mimicking quantum zero point fluctuations (the quantum "half"). Since CS simulations do not know about commutators keeping the zero point fluctuations conserved, this energy is redistributed (incorrectly) to other modes, rather than just appearing as virtual particles for other "real" particles to scatter off. This has led to some confusing interpretations of what are really

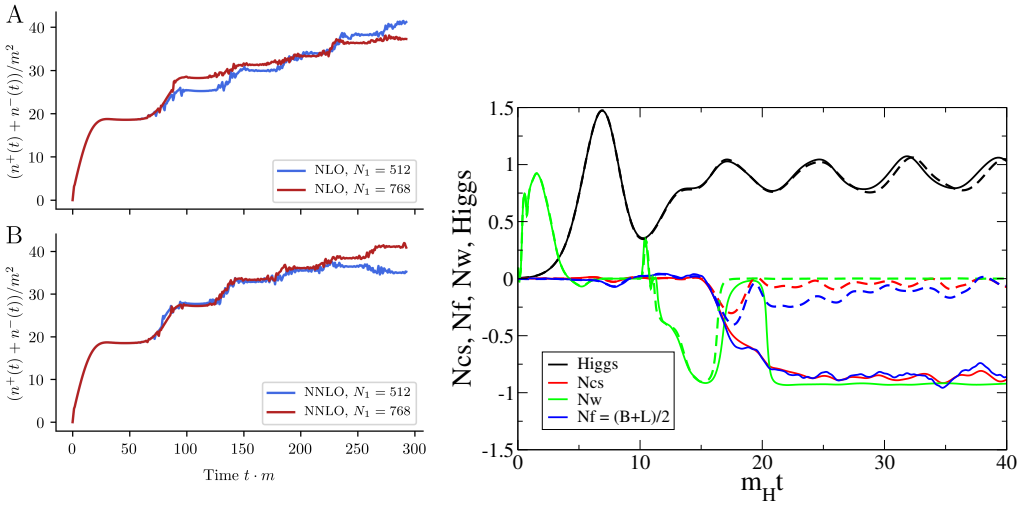

Figure 7: Left: The particle number produced in the Schwinger mechanism. (Reproduced from [11] with kind permission from the authors). Right: The chiral anomaly in a scalar-SU(2)-fermion model of cold baryogenesis (baryogenesis in a tachyonic Higgs transition [12]).

classical simulations (that were subsequently cleared up in [8, 9].

- Truly quantum phenomena such as instantons and tunneling do not occur in CS simulations. Although one may encounter transitions from an ensemble representing a vacuum-like initial conditions, these are classical instances of an out-of-equilibrium initial state jumping over the barrier rather than instanton events [9].

- The CS approximation is well suited for bosonic fields (scalars and gauge fields), that can acquire large occupation numbers. The obvious exception is fermions, which have occupation numbers $n_k \leq 1$. Fortunately, because fermions are bilinear in the action, quantum real time evolution may be implemented in terms of mode functions on classical bosonic backgrounds [10].

$$\psi(x,t) = \int_{k,s} v_s \hat{a}_{k,s} f_{k,s}(x,t). \tag{15}$$

The real-time evolution then amounts to solving a linear evolution equation for the mode functions $f_{k,s}(x,t)$, while correlation functions may be written in terms of these mode functions and the initial conditions for $\langle a^\dagger_{k,s} a_{k,s} \rangle$. Applications include Schwinger pair production Fig. 7 (left, [11]) and the chiral anomaly in the electroweak sector of the Standard Model Fig. 7 (right, [12]).

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

When occupation numbers are not large, or in cases when one is interested in quantum thermalisation also in the UV, the CS approximation is no longer sufficient. One direction, which we will not consider further here is to upgrade the classical evolution equation into a stochastic

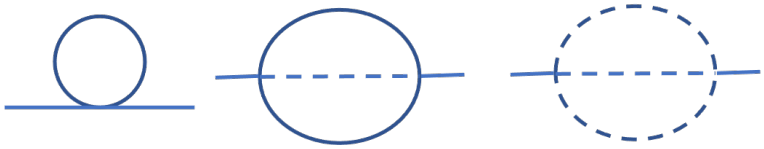

Figure 8: LO and NLO self-energy diagrams in a ϕ^4 theory (where $\bar{\phi} = 0$.

equation. In particular, if there is a natural separation of scales, it is often possible to treat the IR as high-occupation classical fields, while the UV modes retain their quantum evolution. Expanding into mode functions similarly to the fermions above, the UV evolves in the IR long-wavelength background as free fields or interacting fields to some order in perturbation theory (Hard Loops, Hard Thermal Loops, see for instance [13, 14] for examples).

The alternative we will consider here is instead of evolving an ensemble of initial conditions and subsequently averaging, to write down evolution equations for the averages themselves (or quantum expectation values, correlators). This is conveniently phrased in terms of Schwinger-Dyson or Kadanoff-Baym equations, derived from the 2-point irreducible (2PI) quantum effective action. For the technical details, we refer to [15], but in short the 2PI effective action is a generalisation of the standard (1PI) effective action, and a functional of both the 1- and 2-point functions (mean field and propagator). A variational principle allows to derive coupled integro-differential for these quantities, which amount to

$$\left(\partial_t^2 - \partial_x^2 + \hat{M}^2(x)\right)\bar{\phi}(x) = \int_0^{x^0}\int d^3z\,\Sigma^\rho(z,x)\bar{\phi}(z), \tag{16}$$

$$\left(\partial_t^2 - \partial_x^2 + M^2(x)\right)F(x,y) = -\int_0^{x^0} dz^0\int d^3z\,\Sigma^\rho(x,z)F(z,y) + \int_0^{y^0} dz^0\int d^3z\,\Sigma^\rho(x,z)\rho(z,y), \tag{17}$$

$$\left(\partial_t^2 - \partial_x^2 + M^2(x)\right)\rho(x,y) = -\int_{y^0}^{x^0} dz^0\int d^3z\,\Sigma^\rho(x,z)\rho(z,y). \tag{18}$$

The objects $\bar{\phi}$, $F(x,y)$ and $\rho(x,y)$ are the mean field, the statistical and the spectral propagator, respectively. The right-hand sides denote memory integrals over self energies $\Sigma_{\phi,F,\rho}$, that are in turn functions of the ϕ, F, ρ, while the local-in-time part of the self energies are joined with the mass in the objects M^2, $\hat{M}^2$. The equations are explicitly solvable, although numerically challenging. The effective action and the resulting self-energies are truncated through a diagram expansion, and solving the evolution equations amounts to a resummation of diagrams with an in principle infinite number of reinsertions of the same diagrams. Hence a 2PI truncation is an infinite resummation of a particular set of diagrams, leaving out others. As an example, in a NLO truncation of a ϕ^4 theory (with $\bar{\phi}$ taken to vanish by symmetry), the diagrams are shown in Fig. 8.

The selling points and drawbacks of the 2PI formalism include:

- Beyond LO trunctation (when the evolution equations have a non-zero right-hand side), the system equilibrates to a quantum thermal state, including in the UV.

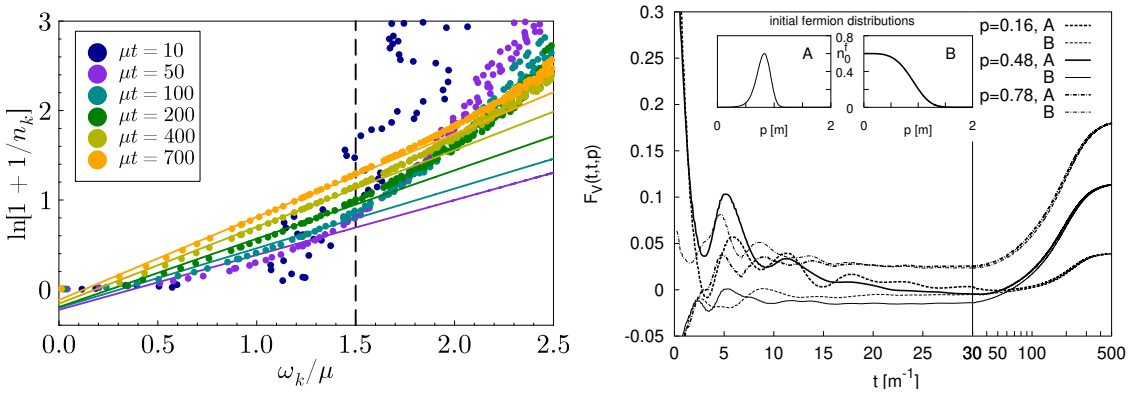

Figure 9: Left: The particle spectrum at different times during tachyonic preheating. (Reproduced from [21]). Right: The time evolution of individual fermion modes in a scalar-fermion model, as the system approaches equilibrium. (Reproduced from [22] with kind permission from the authors).

- There is no requirement of large occupation numbers. Discrepancies with the exact result is down to truncations of the diagram expansions, which are to be controlled by an expansion parameter [16, 17].
- Lattice discretization is straightforward, and allows for numerical solution as a set of coupled differential equations. There is no statistical sampling and hence no statistical error bars.
- Scalar and fermion fields are straighforward to implement, although fermion doublers remain. Gauge fields have technical challenges [18], that are currently being addressed.
- The evolution conserves energy, Goldstone's theorem, (generalised) Ward identities, and the equations are renormalisable [19].
- Since the evolution is based on an (infinitely resummed) perturbative expansion, truly non-perturbative phenomena (such as defects and instantons) may not be correctly included [20].

The formalism has been applied to many out-of-equilibrium phenomena, including:

- Preheating after inflation, Fig. 9 (left, [21]). The figure shows the scalar field spectrum during a tachyonic (spinodal) transition, and subsequent thermalisation. As the process progresses, more and more modes land on a Bose-Einstein-like distribution (straight lines in the figure).
- Thermalisation of scalar-fermion systems, Fig. 9 (right, [22]). The figure shows a set of fermion modes initially in an out-of-equilibrium state. The scalar-fermion system evolves towards the joint equilibrium state, approximately a Bose-Einstein distribution for the scalasr and a Fermi-Dirac distribution for the fermions.

5. Solution #3: Going complex

Finally, for phenomena with small occupation number, and when the perturbative resummations of the 2PI formalism are insufficient (non-perturbative, high precision, beyond (N)NLO), we return

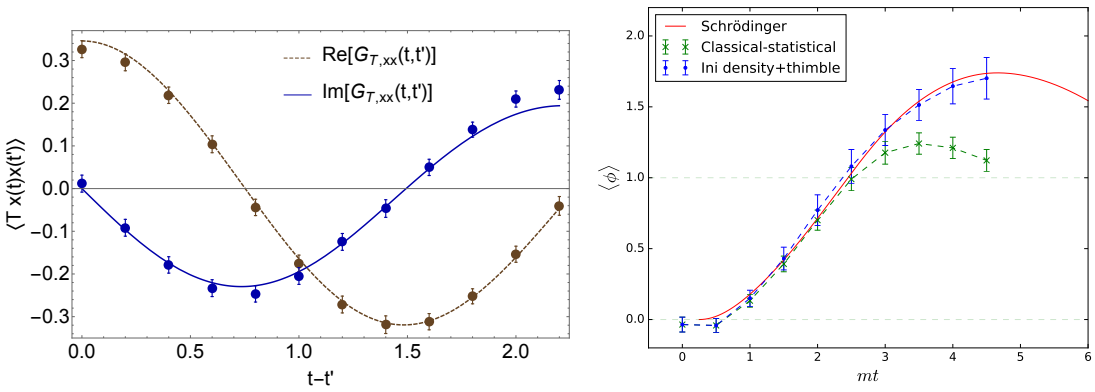

Figure 10: Left: The real-time 2-point function in scalar quantum mechanics. (Reproduced from [24] with kind permission from the authors). Right: The 1-point function in a double well potential, with the system originally in one well at $\phi = 0$. (Reproduced from [25].)

to the evaluation of the path integral itself. As mentioned, the sign problem prevents straightforward sampling, and Wick rotation of the time variable into the complex plane does not work. What is however possible, is to change the domain of integration of the field variables ϕ, by allowing them to take on non-real values.

Thimbles

Perhaps the conceptually cleanest procedure is to deform the real domain (the real axis for each variable, $\mathbb{R}^N$) into some convenient domain of the same dimensionality in the larger complex space $\mathbb{C}^N$. The trick is then to choose this domain, so that the integral converges better (See [23] for a useful review). One option is to use a flow equation to continuously gradually deform $\mathbb{R}^N$ into something better. This is known as a Generalised thimble. Cauchy's theorem (or its generalisation to higher dimension) ensures that the path integral is unchanged for any value of the flow time. Another option is to integrate directly on the optimal manifold, the Lefschetz thimble, for which the integral is known to converge but which may be harder to find and sample on. There may also be multiple thimbles to keep track of. Again, the integral will give the correct result. Both methods are numerical very challenging, and have largely been applied to quantum mechanics at short times, including:

- Computing the real-time 2-point correlator, Fig. 10 (left, [24]). The figure shows the unequal time correlator for an interacting scalar field on 0+1 dimensions.

- Quantum tunneling, Fig. 10 (right, [25]). The figure shows the time evolution of the 1-point function in a double well potential, having been initialised only in one well (around $\phi = 0$). The thimble method is compared to the Schrödinger equation solution and the CS approximation.

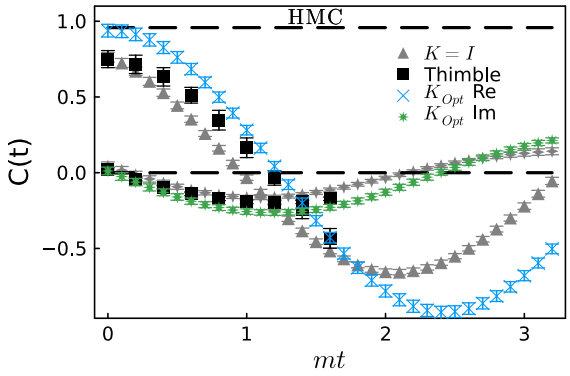

Figure 11: The unequal time correlator in 1+1 dimensional scalar field theory, using complex langevin methods. (Reproduced from [29] with kind permission from the authors).

Complex Langevin

The competing approach is based on stochastic quantization, which for Euclidean systems is a different way of sampling the probability distribution, but giving equivalent results to MC sampling. Given an action, one may write down a (stochastic) Langevin equation that gives an evolution (in auxiliary time), that will eventually probe the correct probability distribution of field configurations. For real-time systems, where iS is indeed complex, a similar procedure will again yield a Langevin equation, which however drives the field variables away from the real axis into the complex plane. Much work has gone into establishing under what conditions this Langevin evolution indeed reproduces the correct distribution [26, 27], and significant progress has been reported, also connecting the Langevin evolution to thimbles. Still, while for non-zero chemical potential there is hope of success [28], for real-time evolution sofar only short physical times have been reached (see Fig. 11, [29]).

6. Summary

Lattice field theory has been a robust and reliable regularization of QFT, which for 50 years has produced groundbreaking physical insight, and precision theoretical input to many areas in high energy physics. The vast majority of work presented at the Lattice conference series concerns equilibrium physics or vacuum-to-vacuum ("zero temperature") matrix elements. But lattice field theory methods are use routinely also on the fringes and beyond the Lattice community, to real-time non-equilibrium evolution of quantum systems, with applications in heavy-ion collisions and early universe cosmology.

Whereas equilibrium computations rely on direct evaluation of path integrals through importance sampling, a severe sign problem prevents the similar implementation for real-time systems. A handful of methods have emerged to deal with these problems, which include: the classical-statistical approximation, which is easy to implement, but misses essential quantum aspects for small occupation numbers; the 2PI/Schwinger-Dyson evolution of correlators, which includes truly quantum effects, but is numerically heavier and based on (resummed) perturbative expansions; and

the evaluation of path integrals allowing complexification of field variables, which is in principle exact but numerically very time consuming and awaiting further developments.

Acknowledgments

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