Symplectic quantization: A new deterministic approach to the dynamics of quantum fields inspired by statistical mechanics*

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Abstract. In this contribution we summarize the main features of a new algorithm (already presented in [1]) to sample numerically on the lattice the quantum fluctuations of fields by means of a deterministic pseudo-Hamiltonian dynamics in an enlarge space of variables. The main goal is to provide a numerical tool which is well defined in Minkowski space. The proposed approach introduces an additional time variable that plays the role of a true physical parameter that controls the deterministic dynamics. The sampling of quantum fluctuations is guaranteed by the presence of new additional conjugated momenta, which represent the rate of variation of ordinary fields with respect to the newly added time variable. From the pseudo-Hamiltonian dynamics one is then able, assuming ergodicity, to retrieve the Feynman path integral as the Fourier transform of a pseudo-microcanonical partition function.

1 Introduction

Since its introduction by Kenneth Wilson [2], lattice field theory has undergone significant advancements [3, 4] as a powerful tool for tackling non-perturbative problems in quantum field theory. This is particularly true for the study of strong interactions, including challenges like the calculation of hadronic masses [5] and the analysis of heavy-ion collisions [6]. However, despite these impressive accomplishments, a fundamental limitation remains: any numerical method on the lattice relies on an importance sampling protocol which is defined only for Euclidean field theory. Yet, while Wick rotation makes numerical approaches feasible, it simultaneously imposes a main limitation: it does not allow for a proper representation of processes that inherently depend on the causal structure of space-time, such as those occurring on the light cone, which is not defined in the Euclidean framework. The probability distribution $\exp(-S_E[\phi]/\hbar)$, to which is mapped in the Euclidean framework the complex phase factor $\exp(iS[\phi]/\hbar)$, essentially acts as an "equilibrium" measure for quantum fluctuations, enabling highly precise reproduction only of stable/equilibrium bound states [5]. However, it fails in capturing metastable resonances with brief lifetimes, such as tetraquark or pentaquark states [7, 8], or the dynamics of relativistic scattering processes, which involve different numbers of degrees of freedom between $\langle \mathrm{IN}|$ and $|\mathrm{OUT}\rangle$ states. For these reasons, we find it crucial to explore numerical tests of any new formulations of quantum field theory that can

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both define and investigate the dynamics of quantum fluctuations directly within Minkowski space-time. A promising idea in this direction is the recent proposal of a functional approach to field theory which is probabilistically well defined also in Lorentzian spacetime. This approach, introduced in [1, 9–11], is referred to as *"symplectic quantization"*. In this framework, for a given quantum field $\phi(x)$, where $x = (ct, \mathbf{x})$ represents a point in four-dimensional space-time, the field is assumed to depend also on an additional time parameter τ, which labels the sequence of quantum fluctuations at each given point of the discretized space-time lattice. An historically well known approach which also makes use of an additional time variable is the Parisi-Wu stochastic quantization approach [12, 13], still well-defined only for Euclidean theories. The use of deterministic dynamics with additional conjugated momenta to model quantum fields fluctuations is also something not new in the literature: it is for instance one of the components of the Hybrid Monte Carlo approach to lattice gauge theory with fermions [14]. But, once more, this has been implemented only for Euclidean theories. The innovative proposal of symplectic quantization, as discussed in [1, 9, 10], is to use the deterministic dynamics to sort quantum fluctuations directly in Lorentzian space-time, by incorporating the conjugate momenta of fields with respect to τ directly into the relativistic action with a Minkowski signature. The idea that some physics can be reproduced only within a microcanonical ensemble approach has been strongly inspired by recent statistical mechanics results for the Discrete Non-Linear Schrödinger Equation, for which the localized phases lives only in the microcanonical [15, 16].

2 The formalism

The symplectic quantization approach to field theory assumes, consistently with the existence of an intrinsic time τ, the existence of conjugated momenta of the kind $\pi(x,\tau) = \dot{\phi}(x,\tau)$ and of a dynamics generated by the following generalized Lagrangian

$$\mathbb{L}(\phi,\dot{\phi}) = \int d^d x \left[\frac{1}{2}\dot{\phi}^2(x) + S(\phi,\partial_\mu\phi)\right],$$

where $S(\phi,\partial_\mu\phi)$ is the standard action for a quantum field, e.g., for a real scalar field,

$$S(\phi,\partial_\mu\phi) = \int d^d x \left(\frac{1}{2}\partial_\mu\phi(x)\partial^\mu\phi(x) - V[\phi(x)]\right) = \int d^d x \left[-\frac{1}{2}\phi\,\partial_0^2\phi + \frac{1}{2}\sum_{i=1}^{d}\phi\,\partial_i^2\phi - V[\phi(x)]\right]$$

where we have integrated by parts and assumed a vanishing amplitude for the field at infinity. Let us then consider the potential $V[\phi(x)] = \frac{1}{2}m^2\phi^2 + \frac{1}{4}\lambda\phi^4$. By means of a Legendre transform, we then pass to the generalized Hamiltonian.

$$\mathbb{H}[\phi,\pi] = \int d^d x \left[\frac{1}{2}\pi^2(x) - S(\phi,\partial_\mu\phi)\right] = \int d^d x \left[\frac{1}{2}\pi^2(x) + \frac{1}{2}\phi\,\partial_0^2\phi - \sum_{i=1}^{d}\phi\,\partial_i^2\phi + V[\phi(x)]\right].$$

We assume that, within the symplectic quantization approach, the dynamics of quantum field theoretical fluctuations is the one governed by the following Hamilton equations:

$$\dot{\phi}(x) = \frac{\delta\mathbb{H}[\phi,\pi]}{\delta\pi(x)} \qquad \dot{\pi}(x) = -\frac{\delta\mathbb{H}[\phi,\pi]}{\delta\phi(x)}, \tag{1}$$

from which we derive the equation of motion for the dynamics of quantum fluctuations:

$$\ddot{\phi}(x,\tau) = -\partial_0^2\phi(x,\tau) + \sum_{i=1}^{d}\partial_i^2\phi(x,\tau) - \frac{\delta V[\phi]}{\delta\phi(x,\tau)}. \tag{2}$$

The effectiveness of symplectic quantization is based on the assumption that the dynamical averages along the trajectories generated by Eq. (1) can be generically replaced by statistical averages over a pseudo-microcanonical ensemble with a partition function built on the conservation of $\mathbb{H}[\phi, \pi]$

$$\Omega(A) = \int \mathcal{D}\phi\mathcal{D}\pi\, \delta\left(A - \mathbb{H}[\phi, \pi]\right) \qquad \rho[\phi(x)] = \frac{1}{\Omega(A)}\, \delta\left(A - \mathbb{H}[\phi, \pi]\right) \tag{3}$$

where ρ is the associated probability density and $\Omega(A)$ a normalisation factor, with $\mathcal{D}\phi$ and $\mathcal{D}\pi$ the standard notation for functional integration. What we mean to say is that, being $\mathbb{H}[\phi(x)]$ a given observable of the quantum fields, symplectic quantization can be related to the standard path-integral formulation of field theory by claiming that for generic initial conditions the following equivalence between ensembles holds:

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T d\tau\, O[\phi(x, \tau)] = \int \mathcal{D}\phi\mathcal{D}\pi\, \rho[\phi(x)]\, O[\phi(x)]. \tag{4}$$

It is in fact possible to see that the Feynman path integral turns out to be nothing but the Fourier anti-transform of the microcanonical partition function written in Eq.(3):

$$\mathcal{Z}(\hbar) = \int_{-\infty}^{\infty} dA\, e^{-iA/\hbar}\, \Omega(A) \propto \int \mathcal{D}\phi\, e^{iS[\phi]/\hbar}, \tag{5}$$

where in the last term of Eq. (5) we have integrated away the quadratic dependence on momenta, which only yields an infinite normalization constant.

3 Numerical simulations

In order to test the effectiveness of our approach, we have run numerical simulations of the theory on a 1+1-dimensional lattice, for which the discretized Hamiltonian reads as:

$$\mathbb{H}[\phi, \pi] = \frac{1}{2} \sum_{\mathbf{i}\in\mathbb{Z}^2} \left[\pi_{\mathbf{i}}^2 + \frac{1}{a^2}\phi_{\mathbf{i}}\Delta^{(0)}\phi_{\mathbf{i}} - \frac{1}{a^2}\phi_{\mathbf{i}}\Delta^{(1)}\phi_{\mathbf{i}} + m^2\phi_{\mathbf{i}}^2 + \frac{\lambda}{4}\phi_{\mathbf{i}}^4 \right],$$

where a denotes the lattice spacing, which has been fixed to $a = 1$, while the symbol $\Delta^{(\mu)}\phi_{\mathbf{i}}$ denotes the discrete one-dimensional Laplacian along the μ-th coordinate axis: $\Delta^{(\mu)}\phi_{\mathbf{i}} = \phi_{\mathbf{i}+\mathbf{e}^{\mu}} + \phi_{\mathbf{i}-\mathbf{e}^{\mu}} - 2\phi_{\mathbf{i}}$. On the 1+1-dimensional lattice the equations of motion Eq. (2) read as:

$$\ddot{\phi}_{n,m}(t) = -\frac{\phi_{n+1,m} + \phi_{n-1,m} - 2\phi_{n,m}}{a^2} + \frac{\phi_{n,m+1} + \phi_{n,m-1} - 2\phi_{n,m}}{a^2} - m^2\phi_{n,m} - \lambda\phi_{\mathbf{i}}^3,$$

where $\phi_{n,m}(t)$ is the field at lattice point with coordinates (n, m).

3.1 Initial conditions

We have shown in Eq. (5) that the Feynman path-integral is connected to the partition function of symplectic quantization by means of a Fourier transform. The partition function $\Omega(\mathcal{A})$ is in turn connected to the Hamiltonian dynamics through an ergodic assumption. It is then legitimate to wonder how to fix the value of $\mathcal{A}$. What we known is that there is a fundamental scale for the "action per degree of freedom", which is $\hbar$. In complete analogy with the definition of temperature in the microcanonical ensemble we can therefore fix the total action $\mathcal{A}$, as suggested in [11], according to the formula:

$$\frac{1}{\hbar} = \frac{d\Sigma_{\text{sym}}(\mathcal{A})}{d\mathcal{A}}.$$

But unless one is able to explicitly compute $\Sigma(\mathcal{A})$, the above relation between $\mathcal{A}$ and $\hbar$ is not particularly useful in practice to assign the value of $\mathcal{A}$. The standard choice to fix $\mathcal{A}$ in order to have $\hbar$ as the typical scale of action is to follow the method of molecular dynamic simulations: fix the energy scale by assigning the appropriate kinetic energy in the initial conditions. Specifically, we ensure that the momentum-momentum correlation is stationary and satisfies $\langle \pi^*(k_i)\pi(k_i)\rangle = \frac{\hbar}{2}$, where k_i denotes discretized momenta. We have therefore set the initial conditions to $|\pi^*(k_i; \tau = 0)|^2 = \hbar$ for all momenta k_i, taking for simplicity $\hbar = 1$. These initial conditions were used for all the simulations presented in this work.

3.2 The role of the non-linearity

It can be easily checked that, in the framework of symplectic quantization, the free theory of a scalar field in Minkowski spacetime is unstable. In fact, considering a quadratic potential $V[\phi] = \frac{1}{2}m^2\phi^2$, we find that in Fourier space the equations of motion reads as $\ddot{\phi}(k,\tau) + \omega_k^2\phi(k,\tau) = 0$, where $\omega_k^2 = |\mathbf{k}|^2 + m^2 - k_0^2$. When $\omega_k^2 < 0$, the solution grows exponentially, leading to an unphysical increase in the field variable. These solutions, which are formally compatible with the conservation of generalized energy, cannot be handled by computers and result, numerically, in an exponential divergence also of the energy, as shown on the right of (Fig. 1). This is due to the accumulation of numerical errors in the algorithm. We observed this behavior using periodic boundary conditions, though they are not ideal for studying causal propagation of signals in the 1+1 lattice. It was then checked numerically that a non-linear attractive potential of the kind $\lambda\phi^4$ prevents the divergence of the free theory, as can be also guessed looking at Eq. (2). The non-linear quartic interaction allows the dynamics to reach a stationary state where energy is conserved within algorithmic bounds, thus allowing the last step of our analysis: the introduction of boundary conditions suitable to study the causal structure of the lattice.

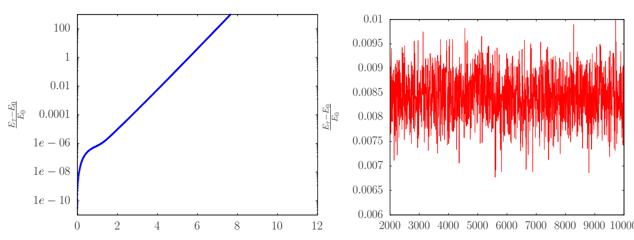

Figure 1. *Behaviour of the normalized energy $(E(\tau) - E_0)/E_0$ vs τ for a scalar theory with $m = 1.0$, $a = 1.0$, $L = 128$. On the left, the theory is free ($\lambda = 0$), and we notice an exponential growth with τ after a short transient. On the right, we added a small self-interaction term, $\lambda = 0.001$. The algorithm is stable with oscillations of order $\delta\tau$.*

3.3 Boundary conditions

An important aspect of this study is the choice of boundary conditions. We used two types of boundary conditions in the simulations. For the stability analysis (Sec. 3.2) we applied standard periodic boundary conditions. However, for the study of signal propagation (Sec. 3.4), we employed *fringe* boundary conditions [17] to simulate an infinite lattice beyond the grid. The fringe boundary conditions consist in adding to the original lattice Γ an external layer Γ_{ext} of tunable thickness, the two forming thus a larger lattice $\Gamma_f = \Gamma + \Gamma_{\text{ext}}$, which we call the *fringe* lattice, to which periodic boundary conditions are finally applied. The main idea of fringe boundary conditions is to have a free transimission of signals at the boundary of Γ and a damping across Γ_{ext}: this effect is achieved by considering different Hamiltonians for Γ and Γ_{ext}. The fringe Hamiltonian is given by $\mathbb{H}_f[\pi,\phi] = \mathbb{H}[\pi,\phi] + \mathbb{H}_{\text{ext}}[\pi,\phi]$ where $\mathbb{H}[\pi,\phi]$ is the original system Hamiltonian and $\mathbb{H}_{\text{ext}}[\pi,\phi]$ includes a damping term to control signal propagation:

$$\mathbb{H}_{\text{ext}}[\pi, \phi] = \frac{1}{2} \sum_{x \in \Gamma_{\text{ext}}} \left[\pi(x)^2 + m^2 \phi(x)^2 + \frac{\lambda}{4} \phi(x)^4 + \alpha \left(\frac{1}{a^2} \phi(x) \Delta^{(0)} \phi(x) - \frac{1}{a^2} \phi(x) \Delta^{(1)} \phi(x) \right) \right],$$

with $\alpha \ll 1$. This setup allows free signal propagation across Γ and damping in Γ_{ext}, ensuring accurate results for the Feynman propagator (Sec. 3.4).

3.4 Results: the Feynman propagator

In this section, we will present numerical evidence showing that for small values of the non-linearity coefficient λ, we qualitatively recover the correct form of the free Feynman propagator. Our approach is straightforward: by setting the non-linear interaction coefficient to a small finite value, $\lambda = 0.001$, we run the symplectic dynamics with fringe boundary conditions until the system reaches a stationary state, let us say at time τ_{eq}. We then study the Fourier spectrum of the two-point correlation function $G(k) = \langle \phi^*(k)\phi(k) \rangle$ by computing the ensemble average as a sliding window average along the dynamics for times larger than the equilibration time, $\tau > \tau_{\text{eq}}$, i.e., according to the definition:

$$\langle \phi^*(k)\phi(k) \rangle = \frac{1}{\Delta\tau} \sum_{i=0}^{M} \phi^*(k, \tau_{\text{eq}} + \tau_i)\phi(k, \tau_{\text{eq}} + \tau_i),$$

where $\tau_i = i \cdot \delta\tau$ and $\Delta\tau = M\delta\tau$. In (Fig. 2), we show (right) the Fourier spectrum of $G(k)$ for $m = 3.0$ and $\lambda = 0.001$, comparing it (left) to the theoretical free Feynman propagator $G_{\text{th}}(k_0, k_1) = \left[\frac{4}{a^2} \sin^2\left(\frac{ak_0}{2}\right) - \frac{4}{a^2} \sin^2\left(\frac{ak_1}{2}\right) - m^2 \right]^{-1}$. The numerical Feynman propagator qualitatively matches the theoretical prediction, exhibiting a saddle shape. The causal structure is even more evident in the real-space correlation function, where we expect undamped oscillations in time-like directions and exponential decay in space-like directions for the Feynman propagator. In fact we should obtain $\Delta_F(x-y) \sim e^{im|x-y|}$ along the time-axis and $\Delta_F(x-y) \sim e^{-m|x-y|}$ along the space-axis. The extracted mass, $m \sim 2.06 \pm 0.04$, differs from the input mass $m = 1.0$, likely due to finite-size effects from the fringe boundary conditions, which we will explore in future works.

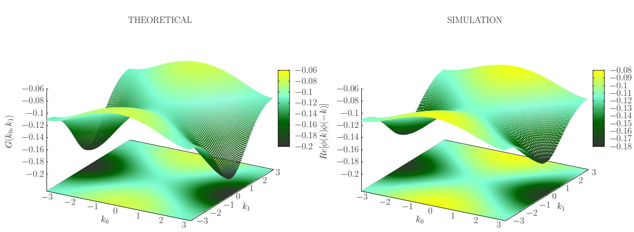

Figure 2. *Real part of the two-point correlation function in Fourier space, for a $\lambda\phi^4$ theory.* ***Left:*** *theoretical value of the free propagator with lattice spacing $a = 1.0$, lattice size $L = 128$, and mass $m = 3.0$.* ***Right:*** *numerical result from the interacting theory $\lambda = 0.001$. No unstable modes are present, meaning $\omega_k^2 > 0$ for all k.*

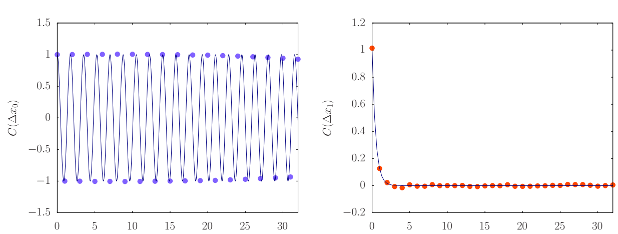

Figure 3. *Two-point correlation function in real space for a $\lambda\phi^4$ theory in $1 + 1$ dimensions with fringe boundary conditions, lattice spacing $a = 1.0$, lattice size $L = 128$, mass $m = 1.0$, and nonlinearity $\lambda = 0.001$.* ***Right:*** *Exponential decay along the x_1 (spatial) axis.* ***Left:*** *Oscillations along the $x_0 = ct$ (temporal) axis.*

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