

Simulating Nonequilibrium Quantum Fields with Stochastic Quantization Techniques

J. Berges¹ and I.-O. Stamatescu^{1,2}

¹*Institute for Theoretical Physics, University of Heidelberg, Philosophenweg 16, 69120 Heidelberg, Germany*

²*FEST, Schmeilweg 5, 69118 Heidelberg, Germany*

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We present lattice simulations of nonequilibrium quantum fields in Minkowskian space-time. Starting from a nonthermal initial state, the real-time quantum ensemble in $(3 + 1)$ dimensions is constructed by a stochastic process in an additional (5th) “Langevin-time.” For the example of a self-interacting scalar field, we show how to resolve apparent unstable Langevin dynamics and compare our quantum results with those obtained in classical field theory. Such a direct simulation method is crucial for our understanding of collision experiments of heavy nuclei or other nonequilibrium phenomena in strongly coupled quantum many-body systems.

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Nonequilibrium quantum field theory is the tool to understand a large variety of topical phenomena in high-energy particle physics, cosmology, as well as condensed matter physics. Current and future collision experiments of heavy nuclei involve far-from-equilibrium dynamics for strongly interacting matter described by quantum chromodynamics (QCD). Other experiments, which have attracted much interest recently, concern the dynamics of ultracold quantum gases. Though these involve length scales many orders of magnitude larger than QCD, they require similar quantum field theoretical techniques.

For out-of-equilibrium calculations, standard approximation techniques, such as perturbation theory, are not uniform in time and fail to describe thermalization. There has been substantial progress in our analytical understanding of nonequilibrium quantum fields using n -particle irreducible functional integral techniques [1]. However, nonequilibrium truncations are difficult to test for crucial questions of QCD or near a Feshbach resonance in atomic media, i.e., where strong interactions play an important role. Direct simulations on a space-time lattice could boost our knowledge and trigger the development of further approximate analytical tools.

Despite the importance of nonperturbative lattice simulation techniques in out-of-equilibrium quantum field theory, these have not been developed so far. This is in sharp contrast to well-established thermal equilibrium methods [2]. Equilibrium calculations can typically be based on a Euclidean formulation, where the time variable is analytically continued to imaginary values. By this, the quantum theory is mapped onto a statistical mechanics problem, which can be simulated by importance sampling techniques. Nonequilibrium problems, however, are not amenable to a Euclidean formulation. Moreover, for real times standard importance sampling is not possible because of a nonpositive definite probability measure. Efforts to circumvent this problem include considering the computer-time evolution in Euclidean lattice simulations [3,4]. A problem in this case is to calibrate the computer time independently of the algorithm.

In this Letter, we present a nonequilibrium quantum field theory simulation in Minkowskian space-time. The quantum ensemble is constructed by a stochastic process in an additional “Langevin-time” using the reformulation of stochastic quantization [5,6] for the Minkowskian path integral [7,8]: The quantum fields are defined on a $(3 + 1)$ -dimensional physical space-time lattice, while the updating procedure employs a Langevin equation with a complex driving force in a 5th, unphysical “time” direction. Nonequilibrium dynamics is implemented by specifying an initial state or density matrix, which deviates from thermal equilibrium. For the example of a relativistic scalar field theory with quartic self-interaction, we compute the time evolution of correlation functions and consider the characteristic damping rates.

Though more or less formal proofs of equivalence of the stochastic approach and the path integral formulation have been given for Minkowski space-time, not much is known about the general convergence properties and its reliability beyond free-field theory or simple examples in equilibrium [8]. Much more advanced applications concern simulations in Euclidean space-time with nonreal actions [9,10], where standard Monte Carlo methods do not work. Despite successful examples, major reported problems concern unstable dynamics and incidences of apparent convergence to unphysical results [9–12].

To our knowledge, the approach has not been used to simulate nonequilibrium quantum field theory before, though some properties seem to make it quite suitable for that. First, nonequilibrium requires specification of an initial state or density matrix. Therefore, the initial configuration is fixed, which seems to stabilize the procedure. Moreover, the additional averaging over an initial density matrix can help to achieve fast convergence. Second, one typically has a good guess for the $(3 + 1)$ -dimensional starting configurations of the Langevin updating procedure: In contrast to the quantum theory, the corresponding classical statistical field theory can be simulated using numerical integration and Monte Carlo techniques [1]. Using the nonequilibrium classical statistical solution as

the starting configuration can improve convergence. It also provides a crucial check of the quantum result in some limiting cases: For sufficiently large macroscopic field or occupation numbers, classical dynamics can provide a good approximation [1].

For our example, we observe good convergence properties of the quantum simulations, which is a remarkable result. For given initial field configurations at time $t = 0$, very different starting configurations for the $(3 + 1)$ -dimensional space-time lattice converge to the same non-equilibrium dynamics for all $t > 0$. To obtain this, we had to resolve the problem of possible unstable dynamics for the updating procedure, as is described in detail below. We compare our quantum results with those obtained for the corresponding classical theory for the same initial conditions and lattice regularization. We indeed find agreement in those cases where this is expected and observe increasing deviations for smaller fields or occupation numbers. In the following, we describe the relevant theoretical ingredients and present the numerical evidence.

Nonequilibrium quantum field theory can be described by the generating functional for correlation functions [1]:

$$\begin{aligned} Z[J; \rho] &= \text{Tr}\{\rho T_C e^{i \int_C J(x)\Phi(x)}\} \\ &= \int d\varphi_1 d\varphi_2 \rho(\varphi_1, \varphi_2) \int_{\varphi_1}^{\varphi_2} [d\varphi] e^{i \int_C (L(x) + J(x)\varphi(x))}. \end{aligned} \quad (1)$$

The path integral (1) displays the quantum fluctuations for a theory with Lagrangian L and the statistical fluctuations encoded in the weighted average with the initial-time density matrix $\rho(\varphi_1, \varphi_2)$. Here T_C denotes contour time ordering along a closed path C starting at $t \equiv x^0 = 0$ with $\int_C \equiv \int_C dx^0 \int d^d x$ (usual time ordering along the forward piece C^+ and antitemporal ordering on the backward piece C^-). The initial fields are fixed by $\varphi_1(\mathbf{x}) = \varphi(0^+, \mathbf{x})$ and $\varphi_2(\mathbf{x}) = \varphi(0^-, \mathbf{x})$. Nonequilibrium correlation functions, i.e., expectation values of Heisenberg field operators $\Phi(x)$, are obtained by functional differentiation. The two-point function, e.g., is

$$\text{Tr}\{\rho T \Phi(x)\Phi(y)\} = \left. \frac{\delta^2 Z[J; \rho]}{i \delta J(x) i \delta J(y)} \right|_{J=0} \quad (2)$$

with all time arguments on C^+ such that T_C corresponds to standard time ordering T . In the following, we consider physical correlation functions, which have their arguments on C^+ . The role of C^- is then only to normalize $Z[J = 0; \rho] = 1$ with $\text{Tr} \rho = 1$.

Complex Langevin.—The complex exponential weight in (1) requires a simulation technique which is not based on a probability interpretation. Stochastic quantization reformulated for real times [7,8] can provide such an approach. The stochastic process is described by a Langevin-type equation, which for a real quantum field theory governs a *complex* field $\phi = \phi_R + i\phi_I$. The appearance of an imaginary part reflects the fact that, in the quantum theory, the field picks up a phase by evolving in time. In addition to the

space-time variable x , the field depends on the Langevin-time parameter ϑ with [7,13]

$$\frac{\partial \phi(x; \vartheta)}{\partial \vartheta} = i \left. \frac{\delta S[\varphi]}{\delta \varphi(x)} \right|_{\varphi \rightarrow \phi} + \eta(x; \vartheta). \quad (3)$$

Here $\delta S/\delta \varphi|_{\varphi \rightarrow \phi} = -\square \phi - m^2 \phi - \lambda \phi^3$ for a scalar theory with mass m and self-interaction λ . In general, the real and imaginary parts of the Gaussian noise term $\eta = \eta_R + i\eta_I$ can be both nonvanishing [8], and the different choices may be used for optimizing convergence. We consider $\eta_I \equiv 0$, with $\langle \eta(x; \vartheta) \rangle_\eta = 0$ and

$$\langle \eta(x; \vartheta) \eta(x'; \vartheta') \rangle_\eta = 2\delta(x - x')\delta(\vartheta - \vartheta'), \quad (4)$$

where $\langle \dots \rangle_\eta$ indicates average over the noise.

The stochastic process (3) is associated to a distribution $P(\phi_R, \phi_I; \vartheta)$, and averages of observables $A(\phi)$ are given as area integrals in the complex field plane:

$$\begin{aligned} \langle A \rangle_\eta &= \frac{\int [d\phi_R][d\phi_I] A(\phi_R + i\phi_I) P(\phi_R, \phi_I; \vartheta)}{\int [d\phi_R][d\phi_I] P(\phi_R, \phi_I; \vartheta)} \\ &= \frac{\int [d\phi_R] A(\phi_R) P_{\text{eff}}(\phi_R; \vartheta)}{\int [d\phi_R] P_{\text{eff}}(\phi_R; \vartheta)}. \end{aligned} \quad (5)$$

Here $P_{\text{eff}}(\phi_R; \vartheta) \equiv \int [d\phi_I] P(\phi_R - i\phi_I, \phi_I; \vartheta)$, where the shift in the integration variable $\phi_R \rightarrow \phi_R - i\phi_I$ for the second equality in (5) is assumed to hold. The complex pseudodistribution $P_{\text{eff}}(\phi_R; \vartheta)$ is indeed governed by the analytic continuation of the Fokker-Planck equation to real times, which admits the stationary solution [7,8]

$$\lim_{\vartheta \rightarrow \infty} P_{\text{eff}}(\phi_R; \vartheta) \equiv P_{\text{eff}}[\phi_R] \sim e^{iS[\phi_R]}. \quad (6)$$

Thus, the approach can, in principle, be used for a Minkowskian theory such as (1), with “ensemble” averages calculated as averages along Langevin trajectories.

Numerical simulation.—We consider $N_s^3 N_t$ lattices with anisotropic space-time discretization a and a_t . Because of the Courant condition, stable dynamics requires $a/a_t \equiv \gamma > \sqrt{d}$. The Langevin-time discretization is $\delta\vartheta$. In terms of lattice variables $\hat{\phi} = a\phi$, $\hat{m} = am$, $\hat{\mathbf{x}} = \mathbf{x}/a$, $\hat{t} = t/a_t$, $\hat{\vartheta} = \vartheta/a^2$, $\epsilon = \delta\vartheta/a^2$, $\hat{\eta} = \sqrt{a^3 a_t} \delta\vartheta \eta = \sqrt{\epsilon/\gamma} a^3 \eta$,

$$\langle \hat{\eta}(\hat{x}, \hat{\vartheta}) \hat{\eta}(\hat{x}', \hat{\vartheta}') \rangle_\eta = 2\delta_{\hat{x}, \hat{x}'} \delta_{\hat{\vartheta}, \hat{\vartheta}'} \quad (7)$$

the discretized Eq. (3) in Itô calculus reads

$$\begin{aligned} \hat{\phi}(\hat{x}; \hat{\vartheta} + \epsilon) &= \hat{\phi}(\hat{x}; \hat{\vartheta}) + \sqrt{\epsilon} \gamma \hat{\eta}(\hat{x}; \hat{\vartheta}) \\ &\quad - i\epsilon [\square_\gamma \hat{\phi}(\hat{x}; \hat{\vartheta}) + \hat{m}^2 \hat{\phi}(\hat{x}; \hat{\vartheta}) + \lambda \hat{\phi}(\hat{x}; \hat{\vartheta})^3]. \end{aligned} \quad (8)$$

Here \square_γ is the (anisotropic) lattice d'Alembertian [14]:

$$\begin{aligned} \square_\gamma \hat{\phi}(\hat{x}) &= \gamma^2 [\hat{\phi}(\hat{x} + \hat{e}_0) + \hat{\phi}(\hat{x} - \hat{e}_0) - c_t \hat{\phi}(\hat{x})] \\ &\quad - \sum_i [\hat{\phi}(\hat{x} + \hat{e}_i) + \hat{\phi}(\hat{x} - \hat{e}_i) - 2\hat{\phi}(\hat{x})], \end{aligned} \quad (9)$$

with $c_t = 2$ for $1 < \hat{t} < N_t - 1$ and $c_{N_t-1} = 1$ for free

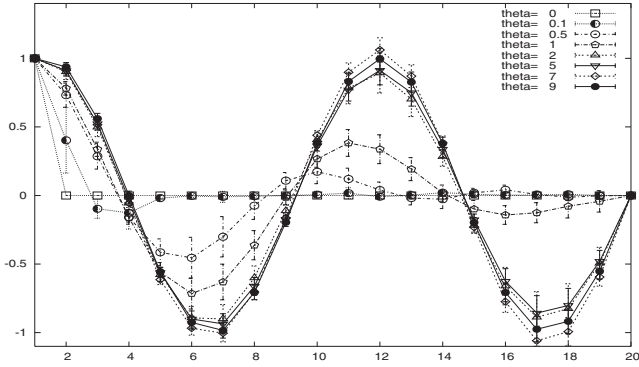


FIG. 1. $\text{Re}C(\hat{t})$ vs \hat{t} for a free-field theory with mass $\hat{m} = 2.315$. The Langevin evolution, shown for $\vartheta = 0-9$ in units of a^2 , converges to the correct result with period $2\pi\gamma/\hat{m}$.

large- \hat{t} boundary conditions (no coupling to $\hat{t} = N_t$). In this case, we consider $\hat{\phi}(\hat{t} = 1, \hat{\mathbf{x}}) = \hat{\phi}(\hat{t} = 2, \hat{\mathbf{x}}) = \hat{\phi}_{\text{class}}(\hat{t} = 1, \hat{\mathbf{x}})$ to set the *initial conditions*. Below, we will also use $c_{N_t-1} = 2$ for fixed large- \hat{t} boundary conditions in the case of a noninteracting field for comparison, and we set $\hat{\phi}(\hat{t} = 1, \hat{\mathbf{x}}) = 1$ and $\hat{\phi}(\hat{t} = N_t, \hat{\mathbf{x}}) = 0$. The classical field configurations $\hat{\phi}_{\text{class}}(\hat{t}, \hat{\mathbf{x}})$ have been obtained by numerically solving the classical field equations and sampling over initial conditions, with nonzero field average and Gaussian fluctuations [1]. Spatial periodic boundary conditions are used.

Here we speak of “initial” configuration, referring to the physical time, and of “starting” configuration for the Langevin process. As *starting* configurations, the classical solution, i.e., $\hat{\phi}(\hat{t} > 1, \hat{\mathbf{x}}; \vartheta = 0) = \hat{\phi}_{\text{class}}(\hat{t} > 1, \mathbf{x})$, or the “null” configuration $\hat{\phi}(\hat{t} > 1, \mathbf{x}; \vartheta = 0) \equiv 0$ are employed. The figures are for a $8 \times 8 \times 8 \times 20$ lattice with $\gamma = 4$ based on 10^6 updatings with $\epsilon = 10^{-5}$ (~ 2 h vector processor time). Error bars are statistical and only indicative.

In the following, we present results for the two-point function (2). In Fig. 1, the correlator

$$C(\hat{t}) = \left\langle \frac{1}{N_s^3} \sum_{\hat{\mathbf{x}}} \hat{\phi}(1, \hat{\mathbf{x}}) \hat{\phi}(\hat{t}, \hat{\mathbf{x}}) \right\rangle \quad (10)$$

for a *free* field of mass $\hat{m} = 2.315$ is shown for fixed boundary conditions with zero momentum initial configuration. $\langle \dots \rangle$ denotes average along the Langevin trajectories [15]. Shown are snapshots of $\text{Re}C(\hat{t})$ for Langevin-time parameter $\vartheta = 0-9$, with null start configuration. The evolution in ϑ exhibits slowly damped oscillations [16], converging to the free-field result with the correct \hat{t} period of $2\pi\gamma/\hat{m}$.

The unequal-time correlator (10) measures the correlation of the field at time \hat{t} with the initial field. It gives important information about the characteristic time scale for the loss of details about the initial conditions. In contrast to the free-field behavior, the interacting theory has a finite characteristic damping time. This is demonstrated in Fig. 2, which shows the connected part

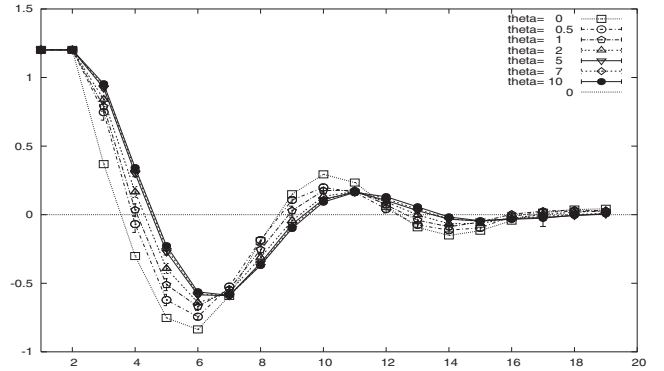


FIG. 2. $\text{Re}G(\hat{t})$ vs \hat{t} for the interacting theory with $\lambda = 1$. As starting configuration ($\vartheta = 0$) the classical result is taken, and the Langevin updating incorporates quantum corrections.

$$G(\hat{t}) = C(\hat{t}) - \left\langle \frac{1}{N_s^3} \sum_{\hat{\mathbf{x}}} \hat{\phi}(1, \hat{\mathbf{x}}) \right\rangle \left\langle \frac{1}{N_s^3} \sum_{\hat{\mathbf{x}'}} \hat{\phi}(\hat{t}, \hat{\mathbf{x}'}) \right\rangle \quad (11)$$

for $\lambda = 1$ and $\hat{m} = 0$. In Fig. 3 a different starting configuration is considered for the same $\hat{\phi}_{\text{class}}(1, \hat{\mathbf{x}})$ initial condition as in Fig. 2. The same data is presented as a function of the Langevin-time ϑ in Fig. 4 to see the convergence. For these parameters, one expects moderate quantum effects. In runs with larger coupling or smaller field, we find that the Langevin updating incorporates increasing quantum corrections. Accordingly, one observes larger deviations compared to the classical starting configuration.

In these simulations with $\epsilon = 10^{-5}$, we encounter incidences of unstable Langevin dynamics (see also [11]). Their appearance depends on the random number and they are strongly suppressed by using a smaller step size, which indicates that they are artifacts of the discretization. To cope with them, we used methods (1) backstepping on the trajectory some thousands of steps (about 0.1 in ϑ) and restart with a new random number and (2) regularizing the process by a small imaginary mass (about $10^{-4}/a$) in the action. Both methods worked quite well. In Fig. 3 triangles

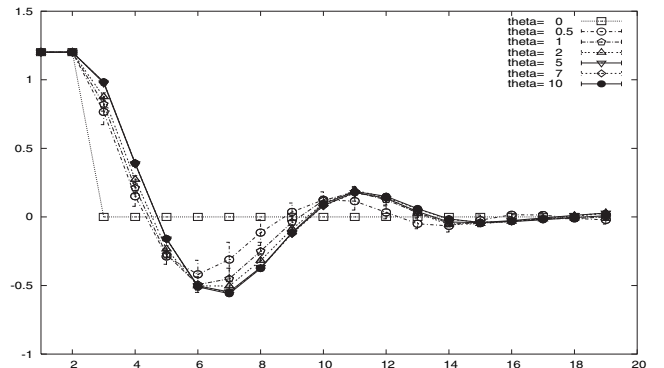


FIG. 3. Same nonequilibrium initial condition as in Fig. 2 but null starting configuration for the Langevin updating. Comparison demonstrates the start independence of the result.

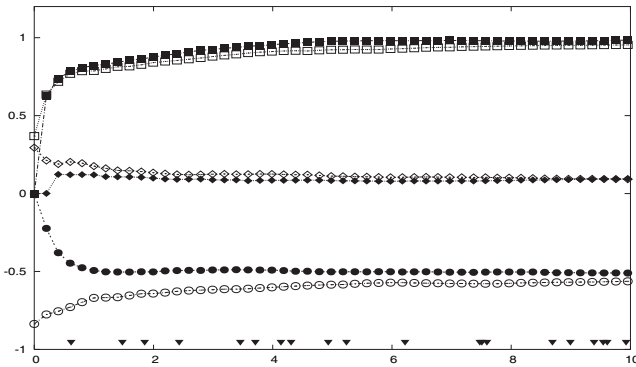


FIG. 4. $\text{Re}G(\hat{t})$ vs \hat{t}/a^2 at $\hat{t} = 3$ (squares), 6 (circles), and 10 (diamonds), for classical (open symbols) and null (solid symbols) starting configurations. Initial conditions as in Fig. 2.

indicate the backsteppings with regularization for the null start. For $\epsilon = 10^{-6}$ we practically could eliminate the “runaway” trajectories on runs of the same \hat{t} length (but tenfold computer time).

Two procedures can be employed for further tests, which are beyond the scope of this Letter. First, one can compare to analytical approximations based on higher n -particle irreducible effective actions [1]. Second, going to sufficiently late times one can compare to certain thermal equilibrium results from Euclidean simulations.

The numerics can be optimized by using improved space-time derivatives and Langevin algorithms. A more systematic study of the convergence problems and of the associated “Fokker-Planck” equation also has to be done. This also includes volume, lattice discretization, and step size dependence, which lead to systematic effects [5–12].

We have demonstrated the possibility of first-principles simulations in nonequilibrium quantum field dynamics. The range of potential applications is enormous. It may be used for out-of-equilibrium as well as Minkowskian equilibrium properties extracted at late times. The scalar theory considered here extended to two components is already relevant for the dynamics of Bose condensates. Possible applications to QCD require implementation in a non-Abelian gauge theory, which is work in progress.

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- [1] J. Berges, in *IX Hadron Physics and VII Relativistic Aspects of Nuclear Physics*, edited by M.E. Bracco, M. Chiapparini, E. Ferreira, and T. Kodama, AIP Conf. Proc. No. 739 (AIP, New York, 2005), p. 3; hep-ph/0409233, and references therein.
- [2] See, e.g., I. Montvay and G. Münster, *Quantum Fields on a Lattice* (Cambridge University Press, Cambridge, England, 1997).

- [3] J.D. Gunton, M. San Miguel, and P.S. Sahni, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J.L. Lebowitz (Academic, New York, 1983), Vol. 8.
- [4] T.R. Miller and M.C. Ogilvie, Phys. Lett. B **488**, 313 (2000); A. Bazavov, B.A. Berg, and A. Velytsky, Int. J. Mod. Phys. A **20**, 3459 (2005); E.T. Tomboulis and A. Velytsky, hep-ph/0507197.
- [5] G. Parisi and Y.-S. Wu, Sci. Sin., Ser. A **24**, 483 (1981); for reviews, see E. Seiler, in *Proceedings of the XXIII Schlading Conference, Austria, 1984* (Springer, Vienna, 1984), p. 259; P.H. Damgaard and H. Hüffel, Phys. Rep. **152**, 227 (1987).
- [6] E. Seiler, I.O. Stamatescu, and D. Zwanziger, Nucl. Phys. **B239**, 177 (1984); **B239**, 201 (1984); G.G. Batrouni *et al.*, Phys. Rev. D **32**, 2736 (1985).
- [7] J.R. Klauder, in *Recent Developments in High Energy Physics*, edited by H. Mitter and C.B. Lang (Springer, New York, 1983); Phys. Rev. A **29**, 2036 (1984); G. Parisi, Phys. Lett. B **131**, 393 (1983); for a review, see K. Okano, L. Schülke, and B. Zheng, Prog. Theor. Phys. Suppl. **111**, 313 (1993).
- [8] H. Hüffel and H. Rumpf, Phys. Lett. B **148**, 104 (1984); E. Gozzi, Phys. Lett. B **150**, 119 (1985); H. Hüffel and P.V. Landshoff, Nucl. Phys. **B260**, 545 (1985); D.J.E. Callaway *et al.*, Nucl. Phys. **B262**, 19 (1985); H. Nakazato and Y. Yamanaka, Phys. Rev. D **34**, 492 (1986); H. Okamoto *et al.*, Nucl. Phys. **B324**, 684 (1989).
- [9] J. Flower, S.W. Otto, and S. Callahan, Phys. Rev. D **34**, 598 (1986); J. Ambjorn, M. Flensburg, and C. Peterson, Nucl. Phys. **B275**, 375 (1986).
- [10] F. Karsch and H.W. Wyld, Phys. Rev. Lett. **55**, 2242 (1985); H. Gausterer and J.R. Klauder, Phys. Lett. B **164**, 127 (1985); Phys. Rev. Lett. **56**, 306 (1986); Phys. Rev. D **33**, 3678 (1986); E.M. Ilgenfritz, Phys. Lett. B **181**, 327 (1986); J. Ambjorn and S.K. Yang, Nucl. Phys. **B275**, 18 (1986); N. Bilic, H. Gausterer, and S. Sanielevici, Phys. Lett. B **198**, 235 (1987); Phys. Rev. D **37**, 3684 (1988); C. Adami and S.E. Koonin, Phys. Rev. C **63**, 034319 (2001); C. Bernard and V.M. Savage, Phys. Rev. D **64**, 085010 (2001).
- [11] J. Klauder and W. Petersen, J. Stat. Phys. **39**, 53 (1985); J. Ambjorn and S.K. Yang, Phys. Lett. B **165**, 140 (1985); T. Matsui and A. Nakamura, Phys. Lett. B **194**, 262 (1987); K. Okano, L. Schülke, and B. Zheng, Phys. Lett. B **258**, 421 (1991); L.L. Salcedo, Phys. Lett. B **305**, 125 (1993); K. Fujimura *et al.*, Nucl. Phys. **B424**, 675 (1994); H. Gausterer, J. Phys. A **27**, 1325 (1994).
- [12] We thank F. Karsch, J. Kogut, and D. Sinclair for discussions about partly unpublished work.
- [13] We do not consider here Nelson’s quantization, which requires no “5th” dimension but needs the ground state wave function to define the driving force of the Langevin dynamics. See, e.g., Seiler [5]. See also T. Hashimoto *et al.*, Nucl. Phys. B, Proc. Suppl. **17**, 723 (1990).
- [14] The updating proceeds sequentially in time and for bushes of independent variables in each time sheet. This improves convergence.
- [15] We note that $\hat{\phi}(1, \hat{x})$ is not updated; therefore, it can be taken out of the brackets.
- [16] These oscillations do not appear in the interacting case.