Numerical Simulation of Ginzburg-Landau-Langevin Equations

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This work is concerned with non-equilibrium phenomena, with focus on the numerical simulation of the relaxation of non-conserved order parameters described by stochastic kinetic equations known as Ginzburg-Landau-Langevin (GLL) equations. We propose methods for solving numerically these type of equations, with additive and multiplicative noises. Illustrative applications of the methods are presented for different GLL equations, with emphasis on equations incorporating memory effects.

Keywords: Mon-equilibrium phenomena; Numerical simulations; Stochastic kinetic equations

I. INTRODUCTION AND MOTIVATION

There are many natural phenomena that occur out of thermodynamic equilibrium and the study of dynamical phase transitions, in particular, is of interest in diverse branches of physics [1]. Among the different aspects of the subject, the understanding of the relaxation of an order parameter is of particular importance. This topic is related to the fundamental question of how a macroscopic irreversible phenomenon like a phase transition arises from a given microscopic reversible dynamics. Answering this question is a very difficult task. In most cases one has to use phenomenological dynamical equations that contain dissipation and fluctuation terms, known as stochastic kinetic equations. Only in rare situations one can derive such an equation starting with a microscopic model. In general, some sort of coarse graining technique has to be used, in which short wavelengths related to microscopic degrees freedom are integrated out in a deterministic equation [2]. This results necessarily in stochastic equations of motion known generically as Ginzburg-Landau-Langevin (GLL) equations.

The traditional GLL equation with additive noise is given by [1]

$$\frac{\partial\phi(x,t)}{\partial t} = -\Gamma\frac{\delta F[\phi]}{\delta\phi} + \xi(x,t) \tag{1}$$

where Γ is an Onsager coefficient, ξ is a noise term and $F[\phi]$ is the Ginzburg-Landau Hamiltonian. In general, $F[\phi]$ is given in terms of a potential $U(\phi)$ as

$$F[\phi] = \int d^3x \left[\frac{1}{2}\gamma(\nabla\phi)^2 + U(\phi)\right] \tag{2}$$

Eq. (1) is a reaction-diffusion type of equation – in the absence of $U(\phi)$ Eq. (1) is precisely the diffusion equation. On general grounds, it is clear that the diffusion equation violates causality – this is also true for Eq. (1). This is so because diffusion processes proceed through a collective motion of matter dominated by microscopic scattering events of infinitely high frequency. In real systems, however, scattering events proceed through finite time intervals and therefore transport memory effects in some circumstances must be taken into account. This is the case for systems in which the time scales of phase conversion are comparable to the microscopic time scales. One example of a system in which the phase conversion is very rapid is the matter formed in high-energy heavy-ion collisions.

Memory effects can be introduced phenomenologically in the GLL equation via a memory function $W(t-t')$

$$\frac{\partial\phi(t)}{\partial t} = \int_0^t dt' W(t-t')\left[-\Gamma\frac{\delta F[\phi(t')]}{\delta\phi(t')} + \xi(t')\right] \tag{3}$$

where we have indicated only the time dependence in the field and noise variables. Now, when the memory function is given by an exponential function of the form

$$W(t-t') = \frac{1}{\alpha}e^{-(t-t')/\alpha} \tag{4}$$

one can easily show that Eq. (3) can be rewritten as

$$\tau\frac{\partial^2\phi(x,t)}{\partial t^2} - \gamma\nabla^2\phi(x,t) \;+\; \eta\frac{\partial\phi(x,t)}{\partial t} + \overline{U}'(\phi) = 0 \tag{5}$$

where we have defined $\overline{U}' = U' - \xi$, and $\tau = \alpha/\Gamma$ and $\eta = 1/\Gamma$. The introduction of memory into the GLL equation brings in the second-order time derivative. Such a second-order time derivative appears naturally in a relativistic quantum field theory of a scalar field. In particular, an effective GLL equation can be obtained by taking into account quantum corrections up to order $\hbar^2$ and second order in the coupling constant, whose general form is given by (in the high-temperature limit) [3]

$$\begin{aligned}\Box\phi(\vec{x},t) \;&+\; \eta\,\phi^2(\vec{x},t)\,\frac{\partial\phi(\vec{x},t)}{\partial t} \\ &+\; U'[\phi,T] = \phi(\vec{x},t)\xi(\vec{x},t)\end{aligned} \tag{6}$$

where $\Box = \partial^2/\partial t^2 - \nabla^2$, and η is the dissipation coefficient associated with the multiplicative noise field ξ given by

$$\eta = \frac{96}{\pi T}\ln\left(\frac{T}{m_T}\right) \tag{7}$$

and m_T is the temperature-dependent mass parameter of the model [3]. Clearly such an equation is of the form of Eq. (5) for $\tau = \gamma = 1$, indicating that it respects causality, which is inherent to a relativistic bosonic equation. There appears also a nonlinear dissipative term proportional to ϕ^2 which gives rise to multiplicative noise term $\phi\xi$, as demanded by the fluctuation-dissipation theorem.

The aim of the present paper is to discuss methods for solving numerically the above equations. Specifically we use two discretization procedures for the spatial coordinates, finite differences and Fourier collocation. For the discretization of the time variable, we use finite differences and leap frog methods. In a separate publication [4] we have performed a numerical analysis for the equations without noise, showing the existence, stability and convergence of the methods for the equations with memory. Here we present results of simulations of the GLL equations with additive and multiplicative noises using the methods developed in Ref. [4].

II. NUMERICAL METHODS - ADDITIVE AND MULTIPLICATIVE NOISE

We divide time in n steps, $t = n\Delta t$, with $n = 0,1,2,\cdots$. Next, we insert the system in a cubic lattice, where $h = L/N$ is the lattice spacing and N is the number of lattice sites in each spatial direction, so that the spatial coordinates (x,y,z) are given by

$$(x,y,z) = (ih, jh, kh) \quad i,j,k \;=\; 0,1,2,....N-1 \tag{8}$$

With this, the field $\phi(x,y,z,t)$ which originally is a continuous quantity becomes discrete and we represent it as ϕ^n_{ijk}. We treat the spatial variables using a Fast Fourier Transform method, so that the field is given by

$$\phi^n_{ijk} = \sum_{rsp=0}^{N-1} a^n_{rsp} E_{rsp}(ijk) \tag{9}$$

with

$$E_{rsp}(ijk) = \exp\left\{ i\frac{2\pi}{Nh} xr + i\frac{2\pi}{Nh} ys + i\frac{2\pi}{Nh} zp \right\} \tag{10}$$

We use two different approximation schemes to handle the Laplacian term, a *finite difference method* (FDM) and *Fourier collocation method* (FCM). In FDM we write the Laplacian term by using finite differences for the spatial derivatives, which leads to

$$\nabla^2 \phi^n_{ijk} \;=\; \sum_{rsp=0}^{N-1} \lambda_{rsp}\, a^n_{rsp} E_{rsp}(ijk) \tag{11}$$

with

$$\lambda_{rsp} = \frac{1}{h^2}\left[-6 \;+\; 2\cos\left(\frac{2\pi}{N} r\right) + 2\cos\left(\frac{2\pi}{N} s\right) \;+\; 2\cos\left(\frac{2\pi}{N} p\right)\right] \tag{12}$$

In the FCM, on the other hand, one simply differentiate the exponential terms in Eq. (10) which leads to a different expression for λ_{rsp}, namely

$$\lambda_{rsp} = \left(\frac{2\pi}{Nh}\right)^2 \left(r^2 + s^2 + p^2\right) \tag{13}$$

In addition, we define the Fourier transform for $\overline{U}' = U' - \xi$ as

$$\overline{U}^n_{ijk} \equiv U'^n_{ijk} - \xi^n_{ijk} = \sum_{rsp=0}^{N-1} b^n_{rsp} E_{rsp}(ijk) \tag{14}$$

With respect to the discretization of the time derivatives, we use two approximation methods, *finite differences* and *leap frog*. In the first method, one has

$$\begin{aligned} \frac{\partial \phi^n_{ijk}}{\partial t} &= \sum_{rsp}^{N-1} \frac{a^{n+1}_{rsp} - a^n_{rsp}}{\Delta t} E_{rsp}(ijk) \\ \frac{\partial^2 \phi^n_{ijk}}{\partial t^2} &= \sum_{rsp}^{N-1} \frac{a^{n+1}_{rsp} - 2a^n_{rsp} + a^{n-1}_{rsp}}{(\Delta t)^2} E_{rsp}(ijk) \end{aligned} \tag{15}$$

In order to simplify presentation, we use an abbreviated notation $k = \{r,s,p\}$. Therefore, using a semi-implicit method in which the Laplacian term is treated at time n, one obtains the following iteration scheme for the Fourier components of the field

$$a^n_k = \frac{(2\tau + \eta\Delta t)\, a^{n-1}_k - \tau a^{n-2}_{rsp} - b^{n-1}_k (\Delta t)^2}{\tau - \gamma\lambda_k (\Delta t)^2 + \eta\Delta t} \tag{16}$$

where λ_k is either given by Eq. (12) for the FDM, or by Eq. (13) for the FCM.

The leap frog algorithm is defined by the iteration scheme

$$\begin{aligned} \dot{a}^{n+1/2}_k &= \frac{[1 - 1/2(\eta\Delta t)]\, \dot{a}^{n-1/2}_k + [\lambda_k a^n_k - b^n_k]\Delta t}{1 + 1/2(\eta\Delta t)} \\ a^{n+1}_k &= a^n_k + \dot{a}^{n+1/2}_k \Delta t \end{aligned} \tag{17}$$

with λ_k again given either by Eq. (12) or Eq. (13) as above.

For the case of Eq. (6), one has multiplicative noise. We deal with this in the following way. Initially we lump together in a single function the derivative of the potential and the noise term and define its Fourier transform as

$$\overline{U}^n_{ijk} \equiv \overline{U}'^n_{ijk} - \phi^n_{ijk}\xi^n_{ijk} = \sum_k d^n_k E_k(ijk) \tag{18}$$

We also define the Fourier transform of the nonlinear dissipative term as

$$\phi^2 \frac{\partial \phi}{\partial t} \to \left(\phi^n_{ijk}\right)^2 \frac{\phi^n_{ijk} - \phi^{n-1}_{ijk}}{\Delta t} = \sum_k c^n_k E_k(ijk) \tag{19}$$

With this, the iteration scheme when treating the time derivatives with a finite difference scheme is given by the equation

$$a^n_k = \frac{2a^{n-1}_k - a^{n-2}_k - \left(\eta\, c^{n-1}_k + d^{n-1}_k\right)(\Delta t^2)}{1 - \lambda_k (\Delta t)^2} \tag{20}$$

When treating the time derivatives with the leap frog algorithm, one has

$$\begin{aligned} \dot{a}^{n+1/2}_k &= \dot{a}^{n-1/2}_k + (\lambda_k a^n_k - b^n_k - \eta c^n_k)\Delta t \\ a^{n+1}_k &= a^n_k + \dot{a}^{n+1/2}_k \Delta t \end{aligned} \tag{21}$$

III. RESULTS OF NUMERICAL SIMULATIONS

In Ref. [4] we have shown that for the one-dimensional case the equations without noise, the methods discussed above are very stable and converge very well with respect to different lattice spacings and time steps. Here we present new results of numerical simulations for the three-dimensional case without and with noise [5]. All results refer to a double-well potential of the form

$$U(\phi) = -\frac{1}{2}\phi^2 + \frac{1}{4}\phi^4 \tag{22}$$

We concentrate here on the time dependence of the volume average of the order parameter, defined as

$$\langle \phi(x,y,z,t) \rangle = \frac{1}{N^3} \sum_{ijk} \overline{\phi}^n_{ijk} \tag{23}$$

where $\overline{\phi}^n_{ijk}$ is the average over a large number N_s of independent noise realizations,

$$\overline{\phi}^n_{ijk} = \frac{1}{N_s} \sum_{s=1}^{N_s} \phi^n_{ijk} \tag{24}$$

The equilibrium value ($n \to \infty$) of this quantity, $\overline{\phi}_{ijk}$, gives the classical average

$$\overline{\phi}_{ijk} = \frac{\int [D\phi]\, \phi_{ijk}\, e^{-\beta F[\phi]}}{\int [D\phi]\, e^{-\beta F[\phi]}} \tag{25}$$

As for the one-dimensional case [4], we found that it is possible to obtain stable, converging solutions for the noiseless three dimensional equations for time steps $\Delta t \leq 0.1$ and lattice spacings $h = L/N \leq 1$. Once $\Delta t \leq 0.1$ and $h \leq 1$, the results are independent of the lattice spacing. In the top panel of Fig. 1 we plot results for the noncausal equation ($\tau = 0$), and in the bottom panel we show the corresponding results for the causal equation ($\tau \neq 0$). The results in this figure are for an initial condition of the form

$$\phi_0(i,j,k) = 0.01 + 0.005\,(2 * \mathsf{ran} - 1) \tag{26}$$

where ran is a random number uniformly distributed in the interval $(0,1)$. For the causal equation, a zero derivative initial condition is used. We present results only for the Fourier collocation method, since the finite difference results are almost indistinguishable from these.

A distinctive characteristic of the solutions in Fig. 1 is the fast exponential growth of the solutions at short times. This is characteristic of the phenomenon of spinodal decomposition [1]. The oscillation after the the spinodal growth in the bottom panel is due to the second order time derivative presented in the causal equation.

The simulation of equations with noise involves some care due to appearance of Rayleigh-Jeans ultraviolet divergences, which manifest themselves in lattice-spacing dependence of the solutions, as shown in Fig. 2 where we show $\langle \phi(x,y,z,t) \rangle$, defined in Eqs. (23) and (24).

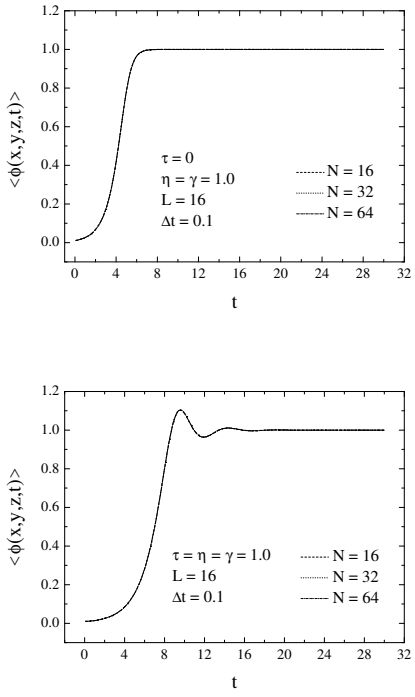

FIG. 1: Volume average of the order parameter as a function of time for different number of lattice sites the Fourier collocation method. Top figure is for the equation without memory and the bottom figure is for equation with memory.

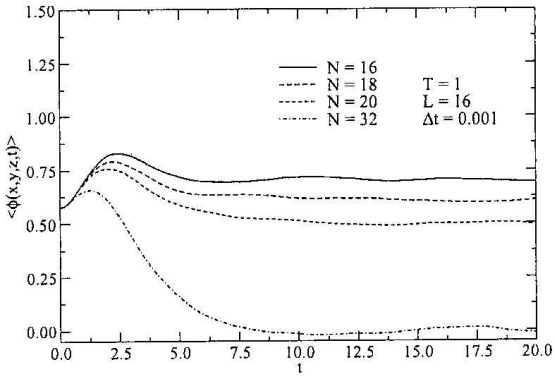

FIG. 2: Solution of the GLL equation with memory with additive noise using the leap frog algorithm for different lattice spacings.

For generating the solutions in Fig. 2 we considered the following initial condition

$$\phi_0(i,j,k) = \frac{1}{\sqrt{3}} + 0.001\,(2 * \mathsf{ran} - 1) \tag{27}$$

with zero first-order derivative. Clearly, the solutions shown in Fig. 2 are not stable as the lattice spacing in varied.

The reason for the divergency of the solutions can most easily be seen from Eq. (24), the functional integral gives divergent perturbative contributions to $\overline{\phi}_{ijk}$ when $U(\phi)$ is of

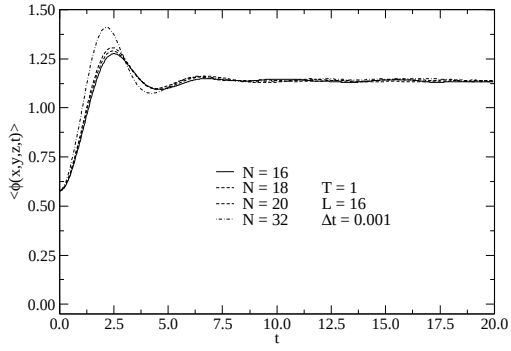

FIG. 3: Solution of the GLL equation with memory and additive noise using the leap frog algorithm for different lattice spacings using counterterms.

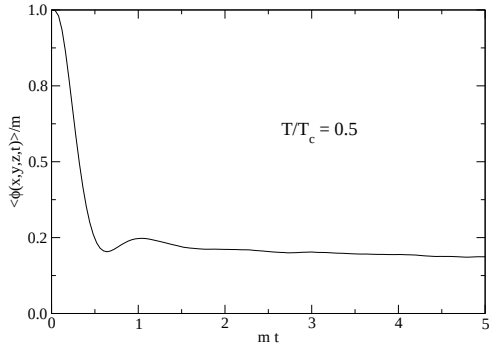

FIG. 4: Solution of Eq. (6) with multiplicative noise using the leap frog algorithm. *m* is the mass parameter in the original Lagrangian Ref. [3].

the form of Eq. (22). One way to handle this instability, at least for obtaining stable equilibrium solutions, is to introduce counterterms in $U(\phi)$. The effective three-dimensional theory is super-renormalizable, since only a tadpole diagram and a setting-sun diagram are divergent and, therefore, to render the theory finite one only needs to subtract from $U(\phi)$ the divergent contributions given by these two diagrams. A more complete discussion on these and explicit expressions for the counterterms can be found in Ref. [6]. In Fig. 3 we present the results of the simulations including the counterterms. One sees that the addition of the regularizing counterterms leads to equilibrium solutions that are independent of lattice spacing.

Finally, we present the result of a simulation using Eq. (6). Our results are shown in Fig. 4 for the broken phase of the model of Ref. [3] with a coupling constant of $\lambda = 0.25$. Note that in this case, the dissipation coefficient η is not a free parameter, but was calculated within the model and given by Eq. (7). We have made several tests regarding sensitivity to lattice spacing and time spacings. The general conclusion is that the time step must be considerably smaller than in the case of the equation without noise. For more details and physical interpretation of results, see Ref. [7].

IV. CONCLUSIONS

In this work we have discussed methods for solving numerically GLL equations in three spatial dimensions with memory effects and additive and multiplicative noises. Specifically we have discussed two discretization procedures for the spatial coordinates, finite differences and Fourier collocation. For the discretization of the time variable, we have discussed finite differences and leap frog methods. We have also pointed out the problem of ultraviolet divergences in the solutions of the GLL equations with noise and discussed a method for obtaining equilibrium solutions that are free from divergences. Explicit solutions were presented for different cases. Most of our attention was on obtaining stable and converging equilibrium solutions.

V. ACKNOWLEDGEMENT

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