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Symplectic integration approach for metastable systems

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Abstract. Nonadiabatic behavior of metastable systems modeled by anharmonic Hamiltonians is reproduced by the Fokker-Planck and imaginary time Schrödinger equation scheme with subsequent symplectic integration. Example solutions capture ergodicity breaking, reassure the H-theorem of global stability [M. Shiino, Phys. Rev. A **36**, 2393 (1987)], and reproduce spatially extended response under alternate source fields.

PACS. 64.60.Cn Order-disorder transformations; statistical mechanics of model systems – 77.80.Dj Domain structure; hysteresis – 77.80.Fm Switching phenomena

1 Introduction

Metastable systems is the active field of study steamed by developments in condensed state physics with model Hamiltonians and relevant Fokker-Planck equations as natural framework of the theory [1]. However, its capacity to reproduce critical phenomena crucially depends on the mathematical technique and in this context the Wentzel-Kramer-Brilluin (WKB) analysis, based on mapping between Fokker-Planck and imaginary time Schrödinger equation, has received a renewed attention [2] and application to systems modeled by anharmonic, nonconservative and nonlocal model Hamiltonians [3,4]. The subject of this work is the development in nonlinear Fokker-Planck — imaginary time Schrödinger equation scheme reproducing critical behavior. Special attention is paid to polarization response in ferroelectrics modeled by Ginzburg — Landau type model Hamiltonians. Unlike the customary direct integration of kinetic equations [5,6] the aforementioned scheme yields a systematic solution of the Dirichlet problem. The paper is organized as follows. In Section 2 we give insight in the Fokker-Planck — imaginary time Schrödinger equation scheme and its application to dynamic hysteresis [7,8]. In Section 3 this scheme is extended for the model of globally coupled anharmonic oscillators reproducing polarization response under alternate source field. In Section 4 the spatial extension and finite size effects are reproduced within the model of locally coupled anharmonic oscillators. The physical background, as well as key problems for further developments, is analyzed in Section 5.

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2 Fokker-Planck and imaginary time Schrödinger equation scheme

The starting point for further generalization is the Fokker-Planck equation for probability density of the order parameter (polarization) $\rho(P,t)$

$$\frac{\partial \rho(P,t)}{\partial t} = \frac{\partial}{\partial P}\left(\frac{\delta U}{\delta P}\rho(P,t)\right) + \Theta\frac{\partial^2 \rho(P,t)}{\partial P^2}. \qquad (1)$$

The (dimensionless) energy functional

$$U = -P^2/2 + P^4/4 + (\nabla P)^2/2 - \lambda(t)\,P, \qquad (2)$$

accentuated in this section emerges from arbitrary model Hamiltonian $H = \int U(\mathbf{P})dV$. The survey hereafter starts with Langevin equation in physical units

$$\frac{\partial P(\mathbf{x},t)}{\partial t} = -\gamma\frac{\delta U[P(\mathbf{x},t)]}{\delta P(\mathbf{x},t)} + \eta(t)$$

subsequently transformed in dimensionless form. Since attention is focused on Ginzburg-Landau type model Hamiltonians, the order parameter P in equation (2) stands for electric polarization. The operator δ means variational derivative of electric polarization as emerged by the gradient term in equation (2) accounting for spatial inhomogeneity in thermodynamic models. However, in equation (1) the entity P appears in standard way as the argument of probability distribution $\rho(P,t)$ returning the expectation value of polarization. The diffusion coefficient Θ comes into play from the Langevin term modeling (additive) fluctuations in Markov-like system. In dimensionless representation equations (1, 2) all specifications of the system are condensed in diffusion coefficient Θ

customary introduced as a noncritical parameter of theory. Developments toward the microscopic interpretation of diffusion coefficient is a problem in quantum-classical boundary [1] and no constructive results have been obtained yet. Considering critical dynamics the standard Fokker-Planck and imaginary time Schrödinger scheme [2] requires that it is possible to divide the spatial domain in decomposed microscopically large blocks modeled by equation (2) so assigning the interaction between blocks separately. To clarify the subtle points in Sections 2, 4 is convenient to consider a single block and ignore integration equation (2) over volume (since rescaling of the diffusion coefficient is not essential). The entity $\lambda(t)$ in equation (2) denotes alternate driving (source) field, and the gradient term $(\nabla P)^2$ specify first neighbor interaction. However, in presence of noise the energy functional equation (2) is not rich enough to reproduce ergodicity breaking and divergence of spontaneous polarization. In this case the probability density of the order parameter equation (1) transforms in a multivariate one and the regular term of equation (1) comprises expectation value of the order parameter. In this sense the problem is nonlinear and its solution involves both a specific mathematical technique and an extension of the model Hamiltonian equation (2).

The essence of the mathematical technique, if applied to an individual block, is to transform equations (1, 2) in imaginary time Schrödinger equation for the auxiliary function $G(P,t)$ introduced by the standard WKB ansatz [2] and unfolding expectation value of polarization through the first moment of probability density $\rho(P,t)$

$$\rho(P,t) = \exp[F(P)]G(P,t). \tag{3}$$

The imaginary time Schrödinger equation is read as

$$\frac{\partial G(P,t)}{\partial t} = \left[\Theta\frac{\partial^2}{\partial P^2} + V(P)\right] G(P,t) \tag{4}$$

and the potential operator $V(P)$ is given by

$$V(P) = \left[\frac{1}{2\Theta}\frac{\partial U(P,t)}{\partial t} - \frac{1}{4\Theta}\left[U'(P,t)\right]^2 + \frac{1}{2}U''(P,t)\right]. \tag{5}$$

The entity $F(P)$ in equation (3) is found as an analytical solution of an ordinary differential equation for so canceling the first derivative of auxiliary function in equation (4) and simultaneously determining the WKB ansatz as

$$\rho(P,t) = \exp[-U(P)/2\Theta]G(P,t). \tag{6}$$

The mapping between equations (1, 4) is quite general and applicable for arbitrary energy functionals. The analytical and quite exact part of computations is completed by recurrence relation for the auxiliary function valid for a small time slice Δt

$$G(P,t+\Delta t) = \exp\left[\Delta t\left(\Theta\frac{\partial^2}{\partial P^2} + V(P)\right)\right] G(P,t). \tag{7}$$

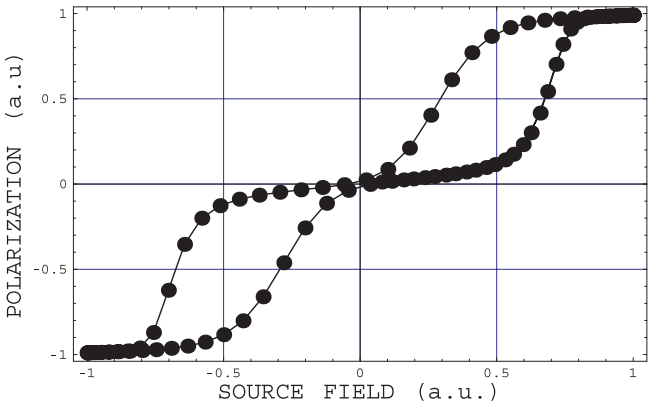

Fig. 1. Dynamic hysteresis plot for $PbTiO_3$ at temperature $T = 1.005\ T_C$, diffusion constant 1/100, and frequency 10^{-3}. The polarization is normalized by the spontaneous one.

The symplectic integrator for equation (7) is read as

$$\left(1 - \frac{\Theta\Delta t}{2}\frac{\partial^2}{\partial P^2}\right) G(P,t+\Delta t)$$
$$= \left\{\exp\left[\frac{\Delta t}{2}V + \frac{\Delta t^3}{48}(\nabla V)^2\right]\left(1 + \frac{\Theta\Delta t}{2}\frac{\partial^2}{\partial P^2}\right)\right.$$
$$\left.\times \exp\left[\frac{\Delta t}{2}V + \frac{\Delta t^3}{48}(\nabla V)^2\right]\right\} G(P,t) \tag{8}$$

and the potential operator V is given with time argument $t := t + \Delta t/2$ [9,10] so accounting for the nonconservative nature of model Hamiltonian. Symplectic integration equation (8) is motivated by its norm conservation and long term stability and, as showed hereafter, applicability to ergodicity breaking and bifurcation of relaxation time as a natural extension of equations (1–8).

Estimates of the nonadiabatic behavior represent one of the classical topics of the theory of metastable systems and are illustrated hereafter by illustrative examples of dynamic hysteresis — the combined effect of periodic source field and additive noise. Dynamic hysteresis plots [3] based on quartic energy functional are in agreement with analytical results [7]. Application of the symplectic integration technique to sixth order energy functional $U(P_1) = \alpha_1 P_1^2 + \alpha_{11} P_1^4 + \alpha_{111} P_1^6$ within the range of metastability is demonstrated in Figure 1. The parameters for $PbTiO_3$ [11] are as follows: Curie-Weiss constant 1.5×10^5 °C, transition temperature $T_C = 492.2$ (°C), $\alpha_1 = 61 \times 10^5$ (m/F) at T_C, $\alpha_{11} = -9.235 \times 10^7$ ($m^5/(C^2F)$), $\alpha_{111} = 3.469 \times 10^8$ ($m^9/(C^4F)$. For model Hamiltonians represented in physical units an entity of interest is the maximum amplitude of the source field (the thermodynamic coercive field) at which the multiwell energy landscape generated by energy functional transforms in a single well one. Fluctuations favor the polarization switching and (in this representative example) a 15% value of the thermodynamic coercive field is sufficient for modeling a

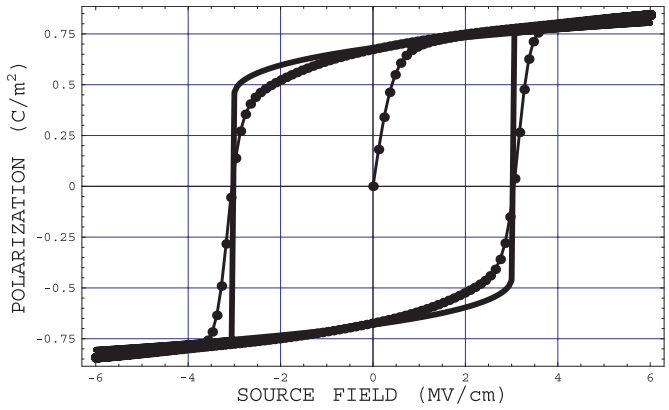

Fig. 2. Comparision of first principle clamped-strain static hysteresis plot for $PbTiO_3$ (bold line) [8] and the polarization response on periodic source (dots). At high frequency source field ($\Omega = 10^{-2}$) the dynamic hysteresis plot approaches to the first principle one and the coercive field resembles the static one, as expected.

hysteresis plot. This value is accepted as a merit for the dimensionless amplitude of the source field represented in Figure 1.

Another illustrative solution demonstrates matching between the statistical and first principles calculations [8] in which the nonlinear dielectric and piezoelectric response of tetragonal $PbTiO_3$ is modeled by energy functional $F(\eta_1, \eta_3, P_z)$ (in denominations of [8]).

$$F = \frac{1}{2}c_{11}(2\eta_1^2 + \eta_3) + c_{12}\left(2\eta_1\eta_3 + \eta_1^2\right) + A_2P_z^2 + A_4P_z^4 + A_6P_z^6 + 2B_{1yy}\eta_1P_z^2 + B_{1zz}\eta_3P_z^2. \quad (9)$$

Here $\eta_1 = \eta_{xx} = \eta_{yy}$ and $\eta_3 = \eta_{zz}$ are components of strain tensor, and the expansion is truncated to the first order in elastic and polarization-strain coupling. Clamped-strain response obtained by zeroing the variations of equation (9) with respect to the components of strain tensor yields renormalization of the expansion coefficient at P^4 in equation (9) as follows [8]

$$F(P_z) = A_2P_z^2 + \left(A_4 + \frac{2c_{12}B_{1zz}B_{1yy} - c_{11}B_{1yy}^2 - (c_{11}+c_{12})\,B_{1zz}^2/2}{(c_{11}+2c_{12})\,(c_{11}-c_{12})}\right)P_z^4 + A_6P_z^6. \quad (10)$$

Since the first expansion coefficient $A_2 < 0$ the energy landscape exhibit two local minima resulting in static hysteresis loop as shown by line in Figure 2. Numerical values of the parameters for $PbTiO_3$ [8] are as follows: $A_2 = -0.003$, $A_4 = 0.005$, $A_6 = 0.004$ (the units for expansion coefficients A_2, A_4, A_6 are m/F, $m^5/(C^2F)$, and $m^9/(C^4F)$). Components of elastic tensor are $c_{11} = 4.374$, $c_{12} = 1.326$, and the coefficients of polarization-strain coupling are equal to $B_{1zz} = -1.99$ and $B_{1yy} = -0.049\ (Nm^2/C^2)$. Modeling of dynamic hysteresis within the scheme equations (1–8) starts with variation of equation (10) and yields Langevin equation (in physical units)

$$\frac{\partial P_z}{\partial t} = -\gamma\frac{\delta\left[F(P_z) - P_z\lambda(t)\right]}{\delta P_z} + \eta(t). \quad (11)$$

Here the parameters of theory are the prefactor (kinetic coefficient) γ, period of source field, and the noise strength $\eta(t)$. At appropriate fitting (diffusion coefficient 1/1000, kinetic coefficient $\gamma = 10$) the dynamic hysteresis plot (dots) match fairly well with the static one.

3 Model of globally coupled anharmonic oscillators

Nonadiabatic behavior of metastable systems under arbitrary driving is a generic problem of physics formally determined by more or less effective model Hamiltonians comprising polarization, polarization-strain coupling, dipole-dipole, driving field, and other terms. The relevant static solutions are well known and are managed with Fourier expansion, variational, and elastostatic Green functions. However, these classical techniques fail in case of critical dynamics, being a highly motivated problem both for physics and technology. Early solutions of this kind have made on the intersection of the theory of complex systems (modeled with quartic potential) and truncated Ginzburg-Landau model Hamiltonians. Some results based on quartic model potential [2,7,15] exhibit a single ground state as a drawback. Advancement, recovering critical phenomena was suggested in [14], however, limited to the case of zero source field. Extension toward arbitrary source field is a problem of mathematical technique managed by symplectic integration. The physical model [14] requires that it is possible to divide the spatial domain in a large number of blocks in such a way that each cell is small enough for all the oscillators in the cell to be assumed to possess the same characteristics of the cell. A set of Langevin equations for the polarization $P(t)$ is read as

$$\frac{\partial P_i}{\partial t} = -\frac{\partial F(P_i)}{\partial P_i} + \sum_{k=1}^{N}\frac{\varepsilon}{N}\left(P_k - P_i\right) + \eta_i(t) \quad (12)$$

here the stochastic terms $\eta_i(t)$ determines additive white noise and the factor $\varepsilon > 0$ denotes the strength of attractive mean-field type coupling. At the thermodynamic $N \to \infty$ limit the averages of P_k in equation (12) can be assumed to behave in a deterministic way, namely,

$$\lim_{N\to\infty}\left(\frac{1}{N}\sum_{k=1}^{N}P_k(t)\right) = \bar{P}(t)$$

and the corresponding Fokker-Planck equation concern probability density for each P_i which originates from

various realizations of white noise

$$\frac{\partial \rho}{\partial t} = \sum_{i=1}^{N} \left[-\frac{\partial}{\partial P_i} \left[-\frac{\partial F}{\partial P_i} + \frac{\varepsilon}{N} \sum_{k=1}^{N} P_k - \frac{\varepsilon}{N} \sum_{k=1}^{N} P_i \right] \rho + \Theta \frac{\partial^2 \rho}{\partial P_i^2} \right]. \quad (13)$$

Recognizing that $\frac{\varepsilon}{N} \sum_{k=1}^{N} P_k(t) = \varepsilon \bar{P}(t)$ and each ith entity concerns a coarse-grained block described by equal kinetics equation (12), the equation (13) reduces to the model of globally coupled anharmonic oscillators

$$\dot{\rho}(P,t) = \frac{\partial}{\partial P} \left[U'(P,t) + \Theta \frac{\partial}{\partial P} \right] \rho(P,t) \quad (14)$$

which generates stationary solutions of equation (14) exhibiting both bifurcation of the ground state (spontaneous polarization) and divergence of the relaxation time for a rich scale of model Hamiltonians. The simplest prototype energy functional comprises the nonlinear term $\bar{P}(t)$ emerging from the mean field coupling, namely

$$U(P,t) = -\frac{P^2}{2} + \frac{P^4}{4} - P\lambda(t) + \frac{\varepsilon}{2} \left[P - \bar{P}(t) \right]^2. \quad (15)$$

The relevant stationary solution is given in [3] and is in agreement with the Boltzmann's H-theorem for global stability (ensuring the existence of a uniquely determined long-time probability distribution $\rho_\infty(P,t)$) and, in case of nonlinearity [14], stating that (at overcritical interaction constant) the system always reaches global stability in the sense that any time dependent solution of equation (14) lying far from equilibrium must be attracted by either one of those stationary solutions without any possibility of runaway behavior or limit cycle type oscillations. Temporal response going beyond this theorem is reproduced in the course of symplectic integration and starts with the ansatz equation (3) that yields relation for the auxiliary function equation (4) $V(P,t) = V_1(P,t) + V_2(\bar{P}(t), P, t)$ made up of both the linear $V_1(P,t)$ and the nonlinear $V_2(\bar{P}(t), P, t)$ terms in the potential operator and explicitly given in [12]. Example solution for a system with initially positive remnant polarization affected by a negative source is demonstrated in Figure 5. The source is modeled by a sow tooth shaped variable length pulse. What is anticipated at $t \to \infty$ limit is approaching the expectation value $\bar{P}$ to a remnant polarization, either P_r or $-P_r$. The sign of the expectation value $\bar{P}$ at the time instant T at which the source turns to zero is crucial, namely, at $\bar{P}(t = T) > 0$ the remnant polarization approaches to $\bar{P}(t = \infty) \to \bar{P}_r$, and $\bar{P}(t = \infty) \to -\bar{P}_r$ otherwise as it follows from the H-theorem of global stability [14]. This behavior is confirmed in Figure 5 with $\bar{P}(T) = 0$ as the point splitting the $\bar{P}$- space in two domains of attraction for P_r and $-P_r$. However, time propagation of the system at $0 < t < T$ within which the source field is nonzero goes beyond the H-theorem of global stability [14] and is revealed in the course of symplectic integration. In this representative solution the source field is

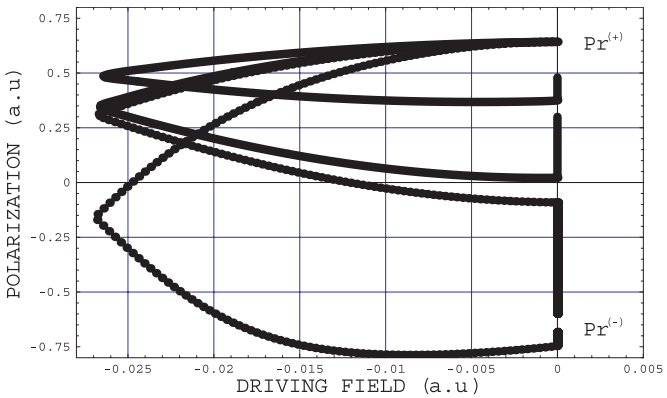

Fig. 3. Temporal response in case of global coupling. Lines illustrate the effect of source pulses being to short (undercritical) for polarization switching and the system remains in the $P_r^{(+)}$ domain of attraction. Otherwise, under pulses with overcritical length (dots) the system enters in the $P_r^{(-)}$ domain of attraction.

specified by -0.027 (a.u.) amplitude (corresponding $\sim$0.07 of the thermodynamic coercive field in physical units) and the pulse length varying between$320 \leq T \leq 1580$ a.u. As shown in Figure 5 the 710 and 1580 (a.u.) source pulses are obviously overcritical and belong to the $-P_r$ domain of attraction. Otherwise, the 320 and 640 (a.u.) source pulses are undercritical and belong to the P_r domain of attraction.

Nonlinearity of this problem is managed by guest function method [12] that has essential consequences for spatially extended problem emerged by locally coupled model in which each anharmonic oscillator is coupled with its first neighbors.

4 Polarization response in the model of locally coupled anharmonic oscillators

Spatial dependence of polarization field, disappearing in the model of globally coupled anharmonic oscillators equations (12), is restored in the case of first neighbors coupling. This approach assumes that (i) the system consist of finite number of (microscopically large) blocks modeled by Ginzburg-Landay energy functional

$$\Phi_i = -\frac{1}{2} P_i^2 + \frac{1}{4} P_i^4 - \lambda(t) P_i$$

(here we consider the $T < T_C$ case and the sixth order term is irrelevant) and (ii) the first neighbor interaction between (macroscopically small) blocks holds so addressing the problem to ensemble of interacting blocks. Going around the microscopic interpretation of the strength of interaction and the correlation length, the problem is formulated by the model Hamiltonian

$$H \equiv \sum_{i}^{N} \left\{ \Phi_i + \frac{\varepsilon}{2} \left(\left(\bar{P}_{i+1}(t) - P_i \right)^2 + \left(\bar{P}_{i-1}(t) - P_i \right)^2 \right) \right\}. \quad (16)$$

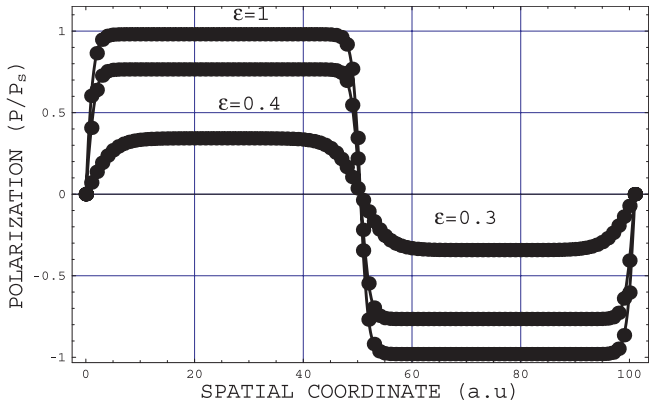

Fig. 4. Stationary solution for 180° domains in a 1-d region with zero boundary conditions and various coupling constants.

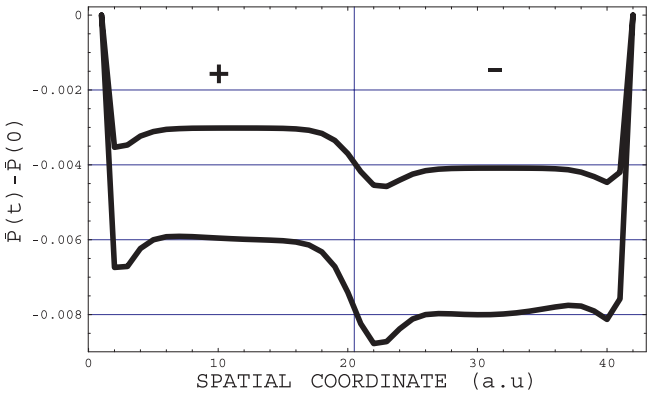

Fig. 5. Effect of negative source field at $t = 26$ and $t = 33$ time instants corresponding to 0.007 and 0.012 of the thermodynamic coercive field. Representative parameters of the problem: first neighbor coupling constant $\varepsilon = 0.035$, diffusion constant $\Theta = 0.05$.

Here the expectation values $\bar{P}_k$ are unknown quantities and are evaluated selfconsistently afterward. Kinetic equations derived from equation (16)

$$\frac{\partial P_i}{\partial t} = -\frac{\partial \Phi_i}{\partial P_i} + \varepsilon\left(\bar{P}_{i+1}(t) - 2P_i + \bar{P}_{i-1}(t)\right) \tag{17}$$

readdress the problem to the set of Fokker-Planck equations for probability distribution

$$\dot{\rho}(P_i,t) = -\frac{\partial}{\partial P_i}\left[-\frac{\partial \Phi_i}{\partial P_i}\rho(P_i,t) + \varepsilon\left(\bar{P}_{i+1}(t) - 2P_i + \bar{P}_{i-1}(t)\right)\rho(P_i,t)\right] + \Theta_i \frac{\partial^2}{\partial P_i^2}\rho(P_i,t). \tag{18}$$

For illustration purpose we consider 1-d Dirichlet problem for two 180° domains. Initial conditions for probability density of polarization are given by stationary solution of equation (18)

$$\rho(P_i) = C\exp\left[\frac{-\Phi(P_i) + \varepsilon P_i(\bar{P}_{i-1} - P_i + \bar{P}_{i+1})}{\Theta_i}\right]. \tag{19}$$

Here C is normalization constant, and $\bar{P}_0 = 0$, $\bar{P}_{i_{\max}+1} = 0$ are zero boundary conditions. Implementing normalization of the probability distribution as well as the first moment $\bar{P} = \int_{-\infty}^{\infty} P\rho dP$ the selfconsistency condition for $\bar{P}_i$ is given by

$$\frac{1}{C}\left(\int_{P_{\min}}^{P_{\max}} P_i \exp\left[\frac{-\Phi(P_i,0) + \varepsilon P_i(\bar{P}_{i-1} - P_i + \bar{P}_{i+1})}{\Theta_i}\right] dP_i\right) - \bar{P}_i = 0. \tag{20}$$

Here C is normalization constant [12]. Initial state of Cauchy problem is given by stationary solution of equation (18) for starting values $\bar{P}_i^{(s)} = 1$ for $i \in [1, i_{\max}/2)$ and $\bar{P}_i^{(s)} = -1$ for $i \in (i_{\max}/2, i_{\max}]$ as demonstrated in Figure 4.

Spatial coordinate emerge from unit size blocks. In total there is a spatial mesh of 100 blocks and the spatial coordinate is paralleled with the number of the block.

Nonstationary solution of equation (18) starts with equation (3) and Fokker-Planck equations equations (22), and yields imaginary time Schrödinger equation for the auxiliary function defined over spatial mesh $i \in [1, i_{\max}]$

$$\dot{G}(P_i,t) = [T[i] + V_1[i] + V_2[i] + K[i]]\, G(P_i,t). \tag{21}$$

Here the kinetic operator $T[i]$ is given by $T[i] = \Theta\frac{\partial^2}{\partial P_i^2}$, the linear part $V_1[i]$ and the nonlinear part $V_2[i]$ of potential operators in equation (28) are given by relations

$$V_1[i] = -\frac{1}{4\Theta_i}\left(\frac{\partial \Phi_i}{\partial P_i}\right)^2 + \frac{1}{2}\left(\frac{\partial^2 \Phi_i}{\partial P_i^2}\right)$$

and

$$V_2[i] = \frac{\varepsilon}{4\Theta_i}\Big(4\Theta_i - \left(2P_i - \bar{P}_{i-1}(t) - \bar{P}_{i+1}(t)\right) \times \left(2P_i - \varepsilon\left(\bar{P}_{i-1}(t) + \bar{P}_{i+1}(t)\right) + 2\frac{\partial \Phi}{\partial P_i}\right)\Big),$$

correspondingly. Finally, correction to the potential operators generated by explicit time dependence of the energy functional yields as $K[i] = [-\varepsilon P_i\dot{\bar{P}}_{i-1}(t) - \varepsilon P_i\dot{\bar{P}}_{i+1}(t) + \dot{\Phi}_i]\,(2\Theta)^{-1}$. Subsequent numerical calculations include the solution of equation (21) and evaluation of the merit $M(Q) = \int P\rho(P,Q,t)dP - (\bar{P}(0) + Q\Delta t)$ (transformed in analytical function of Q_i by quadratic interpolation). This trick generates a set of coupled algebraic equations $M(Q_i) = 0$ for expansion coefficients Q_i so returning the density distributions by equations (3) over spatial mesh in every time slice. Preliminary results of the 1-d domain switching are shown in Figure 5 for a couple of 180° domains Figure 4. Here $\bar{P}(0)$ is the stationary polarization represented in Figure 4. The switching is initiated by a representative negative source field

$\lambda(t) \sim \left[\exp[-(t/150)^2] - 1\right]$ that deviates the value of polarization in both domains. It must be emphasized that the deviation $\bar{P}(t) - \bar{P}(0)$ being negative for any spatial coordinate prevails at the boundaries and at the domain wall in accord with recent estimates [15].

In 3-d case the quantity of interest is 3-d $G(\mathbf{P}, \mathbf{x}, t)$-function which inherits the impact of all components of the polarization vector. However, the general structure of symplectic integration scheme equations (1–8) remains unchanged and its spatial extension is straightforward.

5 Discussion and conclusions

Symplectic integration of nonlinear Fokker-Planck equations capturing Landau-type critical dynamics motivates the analysis of where do the (over)simplified model Hamiltonians constituted from a set of anharmonic oscillators (blocks) stand. Firstly, for globally coupled systems typically each lattice site is connected to all others with the same coupling strength. Physically meaning are microscopically large and macroscopically small objects within which the order parameter is uniform and obey Landau relations. Mutual effect of coupling and noise reproduces both the ordered phase and the ergodicity breaking. Another level of analysis is represented by diffusively coupled blocks located at the sites of a lattice with just nearest neighbor coupling. Formally it yields a generalization of usual thermodynamics for spatially inhomogeneous situations, where the order parameter become a coordinate dependent field $\mathbf{P}(\mathbf{x})$ if smoothed over blocks whose center point lies at $\mathbf{x}$ [1]. An assumption hidden in aforementioned Langevin — Fokker-Planck scheme is that coupling of the constants of theory (prefactor, diffusion coefficient, coupling constant) with the order parameter and other quantities of the theory is not critical. Nevertheless, the symplectic integration approach described here can be extended to more complex Hamiltonians, and to the treatment of multidimensional problems, providing possible directions for future developments of the method.

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