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Brownian motion of particles in 1D arbitrary periodic potentials near a phase transition point

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Abstract. We study the Ambegaokar–Halperin solution of the Smoluchowski equation for arbitrary smooth periodic potentials. Taking into account an analogy between this problem and phase transition phenomena pointed out by Bishop and Trullinger for the harmonic potential, we obtain asymptotic formulae for the mean drift velocity of a particle and find the values of the 'critical exponents', which determine the velocity of a particle. We show that the values of the critical exponents do not depend on potential parameters and they are determined exclusively by analytical properties of the potential. We consider a concrete example of a non-analytical potential leading to other values of the critical exponents.

1. Introduction

The ideas of synergetics—the science studying the dynamics of systems far from equilibrium states—now penetrate into such different fields of science as, for example, instabilities in solids and fluids, chemical reactions, neuron networks [1]. One of the branches of synergetics is studying the dynamics of systems under the influence of stochastic fields. To describe this dynamics in some cases one uses a stationary Smoluchowski equation, which has been applied to an analysis of such phenomena as superionic conductivity, the behaviour of the mean thermal-noise voltage in the Josephson junction, thermally assisted vortex diffusion in superconductors, among others [2].

In all these phenomena there appears a qualitatively new behaviour of systems under the influence of noise as compared to the ideal situation of its absence: namely, the threshold response of a system to applied external forces. Here the noise plays a double role: as a destabilizing and exciting factor for low-energetic states of a system and as a natural limiting factor of the responses of a system to an applied field. An interesting analogy between the unstable behaviour of a nonlinear dissipative system and the thermodynamic phase transition was found in [3]. In the paper of Bishop and Trullinger [4] (BT), it was first noted that the dependence of the mean drift velocity of a particle, moving in a periodic harmonic potential, on temperature T and on an external field F is analogous to the dependence of the order parameter on an external field and on temperature for a classical mean-field phase transition.

Let us recall that the order parameter η in the vicinity of the critical point ($T=T_c$) may be presented in the usual form

$$\begin{aligned} &\eta \sim \begin{cases} \tau^{\beta} & T<T_c \\ 0 & T>T_c \end{cases} \qquad h=0 \\ &\eta \sim h^{1/\delta} \qquad T=T_c \end{aligned} \tag{1}$$

The values of the critical exponents in the context of a classical mean-field phase transition theory are $\beta=1/2$ and $\delta=3$. Here, $\tau=T_c-T$ (T_c is the phase transition temperature, h the external field).

More exactly, BT showed that the velocity of a particle v/F plays the role of an order parameter, $1/F$ plays the role of temperature, temperature T serves as an external field h, and a 'phase transition' takes place at the point where $F=\mathrm{d}U(x)/\mathrm{d}x$ and $\mathrm{d}^2U(x)/\mathrm{d}x^2=0$.

It is interesting for us to describe the above-mentioned systems in the more general situation of an arbitrary periodic field in order to understand how far this analogy may be extended and also to show which potential parameters can be extracted from the experiment.

In our paper it is shown that the indicated analogy may be traced a little further; namely, it turns out that the mean particle velocity displays a universal behaviour, which, in the general case, is not associated with concrete characteristics of the potential. The only important fact is the analytical properties of the potential in the vicinity of the inflection point of the potential $U(x)$. This assertion is based on two simple physical ideas. First, since for continuous phase transitions the critical exponents are independent of the short-range interactions of particles in the system, but are determined by such factors as the interaction symmetry, dimensionality of space and the order parameter, the 'critical exponents' (which determine the velocity of a Brownian particle) should not depend on the form of the potential relief of a moving particle. The second, more concrete idea is based on the assertion that at the 'critical point', i.e. in the case when the external force F is equal to the maximal value of $\mathrm{d}U/\mathrm{d}x$, and temperature T is small in comparison with the characteristic value of the potential U_0, a 'narrow region' of the moving particle is in the vicinity of a point determined as a solution of the equations $\mathrm{d}U/\mathrm{d}x=F$, $\mathrm{d}^2U/\mathrm{d}x^2=0$. The main contribution to the mean drift velocity must be determined by this vicinity. But all functions of a 'general case' in the vicinity of this point x_0 have the same behaviour $U(x)-Fx\simeq U_0+U_0'''(x-x_0)^3/6$ and, hence, they should give the velocity, depending on U_0''' only (see (20), (23) and (24) below).

The outline of the paper is as follows. In section 2 we cite the general solution of the Smoluchowski equation, in section 3 the function $V(x,x')$ inherent in the general solution is analysed, in section 4 we calculate the drift velocity. In section 5 we discuss the obtained results. Finally, some concluding remarks are given in section 6.

2. The Smoluchowski equation and its solution

The diffusion Smoluchowski equation

$$k\frac{\partial\sigma}{\partial t}=\frac{\partial}{\partial x}\left(\sigma\frac{\partial U_t}{\partial x}+T\frac{\partial\sigma}{\partial x}\right) \tag{2}$$

describes the viscous motion of the particle if one neglects the particle inertia. We introduce

$$U(x)=U(x)-Fx \qquad U(x+d)=U(x) \tag{3}$$

where $U_t(x)$ is the total potential, $U(x)$ is periodic in the potential x with period d, F is a driving force and k is a damping constant.

In the stationary case which will be considered below, the Smoluchowski equation for the density distribution function $\sigma(x, t)$ is reduced to the time-independent equation

$$\sigma\frac{\mathrm{d}U_t}{\mathrm{d}x}+T\frac{\mathrm{d}\sigma}{\mathrm{d}x}=-kw \tag{4}$$

where w is an integration constant.

Using the property of the function $f(x)=\exp(-\beta U_t(x))$,

$$\int_0^x \frac{\mathrm{d}x'}{f(x')}=\frac{f(d)}{f(0)}\int_d^{d+x}\frac{\mathrm{d}x'}{f(x')} \tag{5}$$

the solution of (4), satisfying the periodic boundary condition $\sigma(x+d)=\sigma(x)$, can be presented in the form (see [5, 6])

$$\sigma=k\beta w\frac{f(x)f(d)}{f(d)-f(0)}\int_x^{x+d}\frac{\mathrm{d}x'}{f(x')} \tag{6}$$

where now (as distinct from (1)) $\beta=1/T$. Using (4) and the microscopic analogue of the Smoluchowski equation—the Langeven equation

$$k\dot{x}=-\frac{\mathrm{d}U_t}{\mathrm{d}x}+L(t) \tag{7}$$

where $L(t)$ represents the thermally fluctuating Langeven force with zero mean value, we obtain the expression for the mean drift velocity

$$\langle\dot{x}\rangle=dw. \tag{8}$$

The normalization condition for density distribution function $\sigma(x, t)$, $\int_0^d \sigma(x)\,\mathrm{d}x=1$, applied to (6), allows us to find w, and the scaled velocity v

$$v=k\langle\dot{x}\rangle=d[1-\exp(-\beta Fd)]/\beta\Phi \tag{9}$$

normalized so that $v\to F$ at $\beta\to 0$ (see (7) and the definition of Φ (10)). In (9) we introduced

$$\Phi=\int_\alpha^{\alpha+d}\mathrm{d}x\int_0^d \mathrm{d}x'\,\mathrm{e}^{-\beta V(x,x')} \tag{10}$$

$$V(x,x')=U(x)-U(x+x')+Fx' \tag{11}$$

where α is an arbitrary parameter, chosen for the reason of convenience of integration.

3. Analysis of $V(x, x')$

In order to find the drift particle velocity it is necessary to calculate the function Φ in (10). This function has been found by BT for $U(x)=-\cos(x)$. It was shown that v can be expressed by means of a modified Bessel function of imaginary order. In this way, asymptotic expressions for v at different relations between the parameters T, F and U_0' were found. We shall analyse (10) for the arbitrary potential $U(x)$, and particular attention will be paid to the vicinity of the phase transition point $T=0$, $F=U_0'$. Evaluation of the integral (10) may be performed using the Laplace method applied to a two-dimensional region on the plane (x, x'). For this it is necessary to analyse the function $V(x, x')$ and to find the point of its minimum. Silvestr's theorem—the condition of the *minimum of the function* $V(x, x')$—*states that*

$$V_x'=0 \qquad V_{x'}'=0 \qquad V_{xx}''>0 \qquad V_{xx}''V_{x'x'}''-(V_{xx'}'')^2>0. \tag{12}$$

Using (11) we can reduce these expressions to

$$U'(x)=F \qquad U'(x+x')=F \qquad U''(x)>0 \qquad U''(x+x')<0. \tag{13}$$

For simplicity we assume $U(x)$ to be a monotonically increasing function of x at $x_{1m}<x<x_{2m}$, where x_{1m} is the position of the minimum value of $U(x)$ and x_{2m} corresponds to the maximum value of $U(x)$. In addition, without loss of generality, but for the sake of convenience of calculation, let us choose the origin of the coordinates so that at $x=0$ the following relations hold:

$$U_0''=\mathrm{d}^2U/\mathrm{d}x^2_{/x=0}=0 \qquad U_0'=\mathrm{d}U/\mathrm{d}x_{/x=0}>0. \tag{14}$$

With such assumptions the inequality $U_0'''=\mathrm{d}^3U/\mathrm{d}x^3_{/x=0}<0$ is automatically fulfilled, which will be important later.

Let x_1 and x_2 denote the solutions of the equation $U'(x)=F$, for $F<U_0'$. Thereafter, the solutions of (13) are $x=x_1\leqslant 0$, $x'=x_2-x_1$, $x_2\geqslant 0$ (see figure 1). The explicit form of these solutions may be found in the limiting cases: at $F\ll U_0'$ we have

$$x_1=x_{1m}+\frac{F}{U''(x_{1m})} \qquad x_2=x_{2m}-\frac{F}{|U''(x_{2m})|} \tag{15}$$

and at $(U_0'-F)\ll U_0'$, $F<U_0'$ we get

$$x_{1,2}=\pm[2(U_0'-F)/|U_0'''|]^{1/2}. \tag{16}$$

The quadratic minimum of the function $V(x, x')$ determined by (13) exists under the condition $F<U_0'$. With the increase of F from zero to U_0' it is displaced as indicated

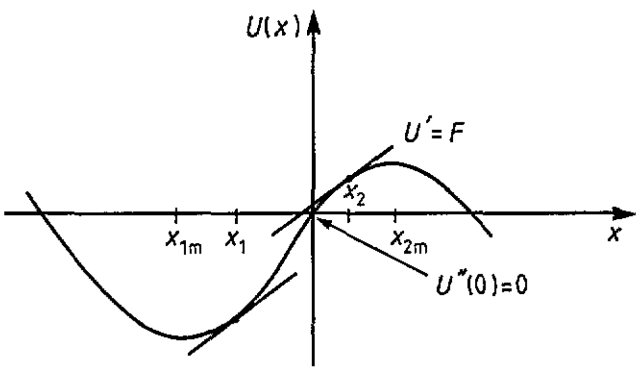

Figure 1. x_1 and x_2 are solutions of the equation $U'(x)=F$.

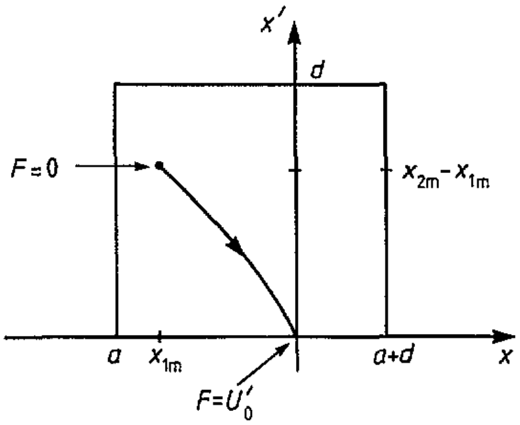

Figure 2. Position of the minimum of the function $V(x, x') = U(x) - U(x+x') + Fx'$. Point A indicates the 'initial' position at $F=0$. With increasing F the minimum point is displaced to position 0, where $F = U_0'$.

in figure 2 from the point $A = (x, x') = (x_{1m}, x_{2m} - x_{1m})$ to the point $(x, x') = (0, 0)$. In the limit $F \to U_0'$ the quadratic minimum disappears and when $F = U_0'$ the expansion of $V(x, x')$ near the point $(0, 0)$ begins with the term of third order. It is also useful to note also the relation $V(x, 0) = 0$. For $F > U_0'$ at the point $(x, x') = (0, 0)$ the derivative $\mathrm{d}V(x, x')/\mathrm{d}x'$ has a minimum value, and this point plays an important role in the integral (10).

4. Calculation of the drift velocity in the vicinity of the phase transition point

For $\beta U_0 \gg 1$ and $F < U_0'$ it is possible to use the Laplace method of calculation of (10). It is convenient to choose the parameter α in (10) so that the boundaries of integration do not pass through the minimum and its vicinity. Expanding $V(x, x')$ in the vicinity of $(x, x') = (x_1, x_2 - x_1)$ with an accuracy of δx^2 and integrating, we obtain from (9)–(11)

$$v = \frac{d}{2\pi}\sqrt{U''(x_1)|U''(x_2)|}[1 - \exp(-\beta F d)\exp[-\beta(U_t(x_2) - U_t(x_1))]. \tag{17}$$

This result is valid if the minimum of the function $V(x, x')$ with its vicinity D, giving the main contribution to the integral (10), does not pass near the boundary of integration, or, in other words, the width D of the distribution function $\sigma(x)$ (see (6)) is less than d and $x_2 - x_1$:

$$D \sim 1/(\beta U'')^{1/2} \ll \mathrm{Min}(d, x_2 - x_1). \tag{18}$$

At $F \lesssim U_0'$ we have $x_1 \sim x_2 \sim d$, and from (18) we get $\beta U_0 \gg 1$. If the difference between F and U_0' is small, i.e. for $(U_0' - F) \ll U_0'$, $F < U_0'$, then using (16), we obtain from (18) $\beta U_0 \gg 1$ and $|\mu| \gg 1$, where

$$\mu = (F - U_0')(6\beta^2/|U_0'''|)^{1/3}. \tag{19}$$

For such values of parameters ($U_0'-F \ll U_0'$, $F<U_0'$ and $|\mu|\gg 1$), the expression for the drift velocity (17) may be simplified with the help of (16), and we get

$$v=\frac{d}{2\pi}\sqrt{2|U_0'''|(U_0'-F)}\,[1-\exp(-\beta F d)]\exp\left(-\frac{2}{\sqrt{3}}|\mu|^{3/2}\right). \qquad (20)$$

For $F\sim U_0'$ and $|\mu|\ll 1$ the position of the minimum is $(x,x')=(0,0)$, and this point gives the main contribution to the integral (10). The coefficients of linear terms in the expansion of $V(x,x')$ near $(x,x')=(0,0)$, under the condition $|\mu|\ll 1$, become small, quadratic terms disappear and the contribution to the integral is determined by cubic terms. Expanding $V(x,x')$ in its vicinity with an accuracy of x^3 and introducing the new variables

$$\begin{pmatrix} x \\ x' \end{pmatrix}=\left(\frac{6}{\beta|U_0'''|}\right)^{1/3}\begin{pmatrix} v-u \\ 2u \end{pmatrix} \qquad (21)$$

we have after integration of (10)

$$\Phi=2\left(\frac{6}{\beta|U_0'''|}\right)^{2/3}\int_0^{\infty} du\,\exp(-2u^3-2\mu u)\int_{-\infty}^{\infty} dv\,\exp(-6uv^2). \qquad (22)$$

For the mean velocity of motion we then get

$$v=\frac{(6/\beta)^{1/3}\,d|U_0'''|^{2/3}}{2[\Gamma(1/3)]^2}\left(1+\frac{2^{2/3}\sqrt{\pi}}{\Gamma(1/6)}\mu\right). \qquad (23)$$

Finally, at $F>U_0'$ and $\mu\gg 1$, as before, the point $(x,x')=(0,0)$ gives the main contribution to the integral (10), because, for all x, $V(x,0)=0$, and the derivative $\mathrm{d}V(x,x')/\mathrm{d}x'|_{x'=0}$ has the minimum value at $x=0$. Using (22) and taking into account $u^3\ll\mu u$, we obtain

$$v=\frac{1}{\pi\sqrt{2}}\,\mathrm{d}\sqrt{|U_0'''|(F-U_0')}\left(1+\frac{15}{32}\mu^{-3}\right). \qquad (24)$$

5. Discussion

We should note first of all that (20), (21) and (24) determine completely the dynamics of a particle in the vicinity of the critical point. To establish the analogy between the obtained expressions and continuous phase transitions, the following correspondence of values will be discussed (see (1)):

Phase transition	η	T	h	T_c
Brownian particle	v/F	$1/F$	T	$1/U_0'$.

For $T>T_c$ and $h\to 0$ an order parameter vanishes: this corresponds to the velocity vanishing in (17) and (20) at $T\to 0$. For $T<T_c$, the power law behaviour of the order parameter τ^{β} at small h corresponds to $v\sim\sqrt{F-U_0'}$ in (24) at $\mu\gg 1$. Finally from (23) one gets $v\sim T^{1/3}$, which is equivalent to the second equality of (1). By analogy we can establish a correspondence between other critical exponents. We do not discuss this problem here since the expressions for other critical exponents coincide completely with those of BT. This coincidence stems from the fact that the results of BT are a particular

case of our results, at least in the vicinity of the critical point. To see this, it is sufficient to substitute $U_0'=1$, $U_0'''=-1$, $F=x$, $\beta=\gamma/2$, $d=2\pi$ in (20), (23) and (24), where the values on the right-hand sides are referred to the notation of BT, and the values of d^nU/dx^n are taken at the inflection point for the potential used by BT, $U(x)=-\cos x$. However, note that the results of BT have a wider range of applicability. This is connected with the fact that in the paper by BT the concrete harmonic potential was used, and the highly developed technique of calculations using Bessel functions allows one to obtain approximate results without the need of such strong inequalities as, for example, $(U_0'-F)\ll U_0'$. Notice also that far from the critical point the velocity is necessarily expressed via the global characteristics of the potential. This naturally diminishes the value of information contained in the formulae, if we deal with the question of reconstruction of potential parameters from experimental data using the above-obtained formulae.

The obtained results can be easily generalized for potentials having a few inflection points on the period. It is clear that in this case there is a 'bottle neck' for a moving particle at the point where the first derivative $U(x)/dx$ is maximal. In this situation it is not difficult to understand that in all the above-mentioned formulae the values of U_0' and U_0''' must be calculated only at the indicated point.

We assumed in our reasoning that the potential $U(x)$ in the vicinity of the inflection point is a smooth function and at this point $U'''\neq 0$. To emphasize the role of the analytical properties of $U(x)$ we consider below the non-analytic piece-by-piece linear potential

$$U(x)=\begin{cases} 2U_0x/d & 0<x<d/2 \\ 2U_0(1-x/d) & d/2<x<d \end{cases} \tag{25}$$

and $U(x)$ repeats itself periodically at $x<0$ and $x>d$. Simple but sufficiently cumbersome manipulations with (9) and (10) give us the following result:

$$v=\frac{4T}{d}\frac{\tilde{F}^2-\tilde{U}^2}{\tilde{F}+2\tilde{U}^2\sinh(\tilde{F}-\tilde{U})\sinh(\tilde{F}+\tilde{U})/[\sinh(2\tilde{F})(\tilde{U}^2-\tilde{F}^2)]} \tag{26}$$

where $\tilde{F}=Fd/4T$, $\tilde{U}=U_0/2T$. In order to compare this result with (23), we consider (26) in the limit $F\to U_0'=2U_0/d$ and $T\to 0$. For the mean velocity v we get from (26) $v=8T/d$. This is evidently different from the result obtained earlier (see (23)). The difference may be understood easily if we take into account that the main contribution to Φ is determined by the region whose dimension δx depends on the character of the potential. For the analytical potential $\delta x\sim T^{1/3}$ (see (22)) each integration with respect to variables x and x' gives $T^{1/3}$. As a result, for the 'cubic minimum' we have (23), where $\Phi\sim T^{2/3}$ and $v\sim T^{1/3}$. A 'bottle neck' for the potential (25) does not depend on T, $\delta x=d/2$, and we get $\Phi\sim T^0$ and $v\sim T$.

To obtain further insight into the problem, we want to point out another way of calculating (26) at the critical point. Figure 3 shows the function $V(x,x')$ for the potential (25) in the case $F=U_0'=2U_0/d$ (cf. figure 4). We can see that in the limit $\beta\to\infty$ the function Φ is equal to $d^2/8$ (see (10) and figure 3). From (9), in the same limit $\beta\to\infty$ we get $v=d/\beta\Phi$, and finally we have the above-mentioned result $v=8T/d$.

To explain in more detail the connection of the two results (23) and (26), by means of the limiting procedure we shall study qualitatively another potential which gives such

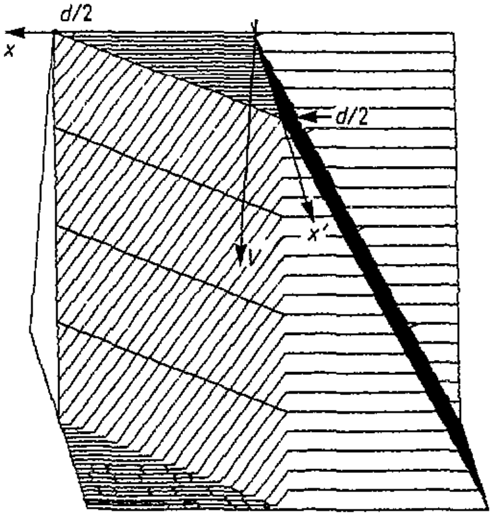

Figure 3. The function $V(x, x')$ for the piece-by-piece linear potential (25) for the case $F = U_0' = 2U_0/d$.

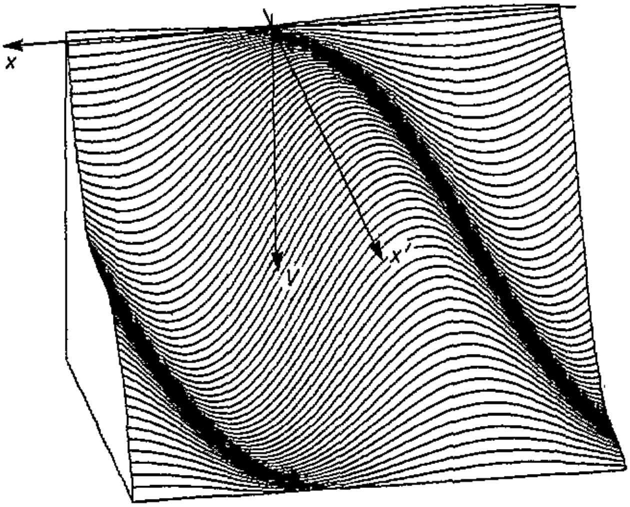

Figure 4. General view of the function $V(x, x')$ for the smooth potential $U(x)$ in the vicinity of the point (0, 0) for the case $F = U_0'$.

a possibility. We consider the potential $U(x)$ defined in the following way:

$$U(x) = U_0 \sin[\pi(|x| - d/4)/L] \qquad |x| < d/2 \tag{27}$$

which repeats itself periodically for $|x| > d/2$. For $L = d/2$ it gives the analytical potential $U(x) = -U_0 \cos(2\pi x/d)$. In the limit $L \to \infty$ it coincides with the non-analytic potential (25), i.e. it gives the possibility of studying the limiting transition from the result (23) to the case of the non-analytical potential (25) when $L \to \infty$. For the potential (27) we have $U_0''' \sim U_0/L^3$, $\delta x \sim (1/U_0'''\beta)^{1/3}$ and from $\delta x \ll d$ we get the condition of applicability of (23), namely $L \ll d(\beta U_0)^{1/3}$. With increasing L the region on the plane (x, x') making the essential contribution to the integral (10) grows. The cubic maximum in the vicinity (0, 0) (see figure 4) is transformed into a plane three-angular region of figure 3. In the case of the strong inequality $L \gg d(\beta U_0)^{1/3}$, when the third derivative U_0''' becomes abnormally small we come to the potential (25) and to the result $v \sim T$. However, it is very difficult to calculate Φ in the intermediate case $L \sim d(\beta U_0)^{1/3}$.

6. Conclusion

In this paper the movement of a Brownian particle in the arbitrary periodic potential under the influence of a constant external force is considered. It is shown that the character of the movement of the particle in the vicinity of the critical point does not depend on the form of the potential, but it is determined by its analytical properties in the vicinity of the potential inflection point. Thus, an analogy between Brownian motion and continuous phase transitions takes place not only for the harmonic potential. Undoubtedly, such an analogy might be more interesting with the fluctuation phase transition theory. We hope it may be realized in the framework of more complicated models; for example, in the nonlinear sine–Gordon chain considered in [7]. Despite many theoretical works in this direction [8–14] (see also [15] and the numerous references therein), the behaviour of the sine–Gordon chain in the vicinity of the critical point still remains unexplored. We intend to present the results of studying these systems in future publications.

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