Application of the Statistical Physics Methods
for the Investigation of Phase Transitions
in the Lotka–Volterra System with
Spatially Distributed Parameters

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Abstract

The application of statistical physics methods for the investigation of phase transitions for a generalization of the Lotka–Volterra system with additional terms that take into account the spatial distribution of species is considered. The additional terms are chosen in such a way that the generalized system, as well as the classical Lotka–Volterra system, is Hamiltonian. Kerner's approach, who was the first to use statistical mechanics for the analysis of Hamiltonian Volterra-type systems, is used to investigate the generalized Lotka–Volterra system. In addition, the Lee–Yang approach is used to calculate zeros of the statistical sum. The position of these zeros is used to find out whether there are phase transitions in the model under examination.

Keywords: Lotka–Volterra system, statistical sum, gamma function, Lee–Yang zeros

1. Introduction

It has been shown (e.g., see [4], [22], [25], [26], [28], [29], [30] [31]) that in some ecological and biological systems processes similar to phase transitions in statistical
physics are observed. In such systems, qualitative changes occur similarly to the statistical and thermodynamic changes that are observed in phase transitions in statistical physics. Examples of such processes that have not yet found a proper scientific explanation are as follows:

– Qualitative changes in forest ecosystems in the course of ecological succession when, e.g., a deciduous forest is replaced by coniferous forest and (or) a community of herbaceous plants is replaced by a community of woody plants.
– Bursts of mass reproduction of lemmings in tundra zone accompanied by their migration from the habitat and mass mortality. As a result, the population of lemmings first significantly decreases and then gradually increases up to the new burst of mass reproduction.
– Periodically repeating bursts of mass reproduction of forest insects.
– Phase transitions in biological membranes accompanied by the transition from the liquid crystal state to the solid crystal state and vice versa.

In this paper, we apply methods and approaches of statistical physics for the analysis of phase transitions in ecological and biological systems. The choice of statistical physics methods and approaches is explained by the fact that during many years of the development of statistical physics, a vast amount of experimental and theoretical data that make it possible to solve complicated problems have been accumulated.

The theory of phase transitions is an important branch of statistical physics. The theory of phase transitions and related critical phenomena has a rich history. Many prominent physicists, both theorists and experimenters, contributed to the development of the theory of phase transitions. Even though the first significant studies of critical phenomena in various substances appeared as early as in the second part of the 19th century, the development of this division of the statistical physics continues.

Studies go on in various divisions of physics, and the accumulated data are steadily updated. The mathematical methods are elaborated, and advanced devices are used that improve the accuracy of experiments.

Presently, the modern statistical physics has a variety of methods, approaches, and theories that make it possible to describe, analyze, and understand the essence of the processes and critical phenomena that occur during phase transitions in various systems (see [1], [2], [6], [7], [8], [9], [12], [17], [20], [21], [23], [27], [43], [48], [49], [50], [52], [54], [55], [56], [57]).

The large number of methods, approaches, and theories is explained by the complexity and diversity of phase transitions and critical phenomena that cannot be explained using a unified theory or approach.

The first theory used a hundred years ago to theoretically describe critical phenomena was the mean field theory.

Among the mean field theories are the Gibbs critical point theory [18], [19], the Weiss theory of ferromagnetism, and the Landau theory of phase transitions of the second kind [44], [45].

The mean field theory turned out to be inapplicable when fluctuations become significant, i.e., in the vicinity of the point of phase transition.
The fluctuation theory of phase transitions of the second kind [53] describes the interaction of fluctuations, makes it possible to take into account the interaction of fluctuation phenomena at critical points, and determine the values of critical parameters.

The microscopic theory of phase transitions makes it possible to investigate the properties of concrete models that undergo a phase transition. The main difficulty in the development of the microscopic theory of phase transitions is the absence of an explicit small parameter.

Recently, quantum phase transitions have been widely studied (see [24], [41], [42], [71]); transitions of matter from one quantum thermodynamic phase into another under changes of the external conditions in the case when there are no thermal fluctuations are investigated.

An important step in the history of the development of phase transition theories are the theories that appeared in the 1960s and 1970s, which enriched the statistical physics by the concepts of renormalization group, scale invariance, and universality (see [10], [11], [13], [14], [15], [16], [33], [34], [35], [36], [64], [65], [66], [67], [68], [69], [72]).

Using the coarsening techniques, these methods provide a tool for the analysis of such difficult physical problems as quantum field theory and the theory of critical phenomena.

The renormgroup divides the ferromagnetic system in the vicinity of a critical point into cells of which each contains a small number of atomic-level magnets; the size of cell determines the scale. This method made it possible to describe the behavior in the vicinity of the critical point and obtain a quantitative estimate of the properties of the system under examination on a computer.

The scale invariance is the property of the equations describing a physical theory or process to remain invariant when all the distances and time intervals are multiplied by the same factor.

**A large number of model systems are used in statistical physics to describe and investigate phase transitions and critical phenomena.** Such models include lattice magnetic models, such as two-dimensional and three-dimensional Ising models, Heisenberg's model, Matsubara and Matsuda models, Stanley $n$-component models, spherical Berlin and Kac model, lattice percolation model used to investigate complex systems, the lattice gas model for the description of the liquid–vapor critical point, and others.

Among them, the Ising model, which is widely used for the investigation of phase transitions, deserves special attention. This model was designed for the investigation and description of ferromagnetic phenomena. Ising claimed in 1924 (see [32]) that there are no phase transitions in one-dimensional systems and the one-dimensional lattice does not exhibit ferromagnetism.

In 1942, Onsager obtained an exact solution for the two-dimensional Ising model [51].

**One of the first researchers who applied the methods and approaches of statistical physics for the investigation of biological models was the American physicist E.H. Kerner.** Beginning from 1957, he published a series of papers [37],
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[38], [39], [40] devoted to the application of statistical mechanics methods for the analysis of Volterra-type models. Using the features of these systems, Kerner developed for them analogs of the main thermodynamic parameters, such as internal energy, entropy, and statistical sum. Kerner explicitly calculated the statistical sum for the Lotka–Volterra equation. He also discovered a remarkable feature of the Hamiltonian of the Lotka–Volterra system. This is the fact that the statistical sum for this system can be calculated explicitly in terms of the gamma functions up to a factor representable in terms of the elementary functions. Kerner's studies confirmed the possibility and usefulness of applying the statistical mechanics methods to the analysis of Volterra-type equations.

In addition to Kerner's studies, the methods of statistical physics were used for the investigation of biological and ecological models in [3], [5], [58], [59], [60].

**In this paper, we want**

– to use the result of theoretical and experimental studies of phase transitions and critical phenomena obtained in statistical physics for the investigation of phase transitions in biological and ecological systems by finding an appropriate simple mathematical biology model;

– to find a calculation method and use mathematical transformations and approximations that would enable us to obtain the result as easily as possible (practically manually) without using long and complicated computer calculations;

– to obtain an analytical solution that would enable us to determine graphically whether there is a phase transition in the system.

**The aim of this paper is** to develop an approach that provides simple means for determining whether there is a phase transition in the system.

**For the investigation of qualitative changes in biological and ecological systems** that resemble phase transitions in physical systems, we use a generalization of the classical Lotka–Volterra model [47], [61], [62], [63] in which terms taking into account the spatial distribution of species are added.

**As the investigation techniques, we use the approach of Kerner, who was the first to apply statistical physics methods for the analysis of Volterra systems, and the Lee–Yang approach** [46], [70], which allows one to detect the existence of phase transitions from the position of zeros on the complex plane.

**The thermodynamic state and properties of the system are studied using the statistical sum**, which is represented in terms of a simple combination of elementary and gamma functions. The existence and nonexistence of phase transitions is determined based on the position of the zeros of the statistical sum on the complex plane.

The paper is organized as follows:

1. Introduction.
2. The description of the investigation techniques and features of the model.
3. Calculation of the statistical sum for the model under examination.
4. Investigation of the phase transition in the model.
5. Conclusions.
2. The description of the Investigation Techniques and Features of the Model

2.1. The Investigation Technique

We use the approach of Kerner [3], [38], [39], [40], who was the first to apply statistical mechanics methods for the analysis of Volterra systems. Kerner used a change of variables that allowed him to calculate the statistical sum in terms of the gamma functions accurate to elementary functions. Kerner applied the change of variable directly to the whole statistical sum. In this paper, we cannot apply Kerner’s approach directly because in our case we have extra terms added to the classical Lotka–Volterra system that take into account the spatial distribution of species. This considerably complicated the equations under examination. To overcome this difficulty, we expand the statistical sum into Taylor’s series and apply Kerner’s change of variable to each term of this series, which has a proper form. In this case, each term is represented by a combination of the gamma functions and elementary functions. Then, the series is summed to obtain the final statistical sum.

The existence or nonexistence of phase transitions in the system is determined graphically judging by the position of the zeros of the statistical sum on the complex plane.

2.2. A Description of the Model Features

The classical Lotka–Volterra system has the form

$$\frac{d\phi}{dt} = \phi - \phi \psi, \quad \frac{d\psi}{dt} = -\psi + \phi \psi. \quad (2.2.1)$$

Here $\phi$ is the population of prey, and $\psi$ is the population of predators.

The classical Lotka–Volterra system does not take into account the dependence of the species of predators and prey on spatial coordinates. Taking into account this dependence can considerably improve the analytical power of the model. To take the spatial dependence into account, we denote the flows of predators and prey by $j_1$ and $j_2$, respectively. The generalization of the Lotka–Volterra system with account for the spatial dependence of the predator and prey population has the form

$$\frac{d\phi}{dt} = \phi - \phi \psi + \text{div}j_1, \quad (2.2.2)$$

$$\frac{d\psi}{dt} = -\psi + \phi \psi + \text{div}j_2. \quad (2.2.3)$$
The contribution of the predator and prey population to time derivatives is determined by the divergences of the flows $j_1$ and $j_2$. We assume that the flow $j_1$ is equal to the gradient of the predator population $\psi$ with the opposite sign:

$$j_1 = -\nabla \psi .$$  \hspace{1cm} (2.2.4)

The interpretation is that the prey tend to the place where the population of predators is lower. Similarly, we assume that the flow of predator population $j_2$ equals the gradient of the prey population $\phi$:

$$j_2 = \nabla \phi .$$  \hspace{1cm} (2.2.5)

This means that the predators tend to the place where the prey is more numerous. Under these assumptions, the generalization of the Lotka–Volterra system takes the form

$$\frac{d\phi}{dt} = \phi - \phi \psi - \Delta \psi ,$$  \hspace{1cm} (2.2.6)

$$\frac{d\psi}{dt} = -\psi + \phi \psi + \Delta \phi .$$  \hspace{1cm} (2.2.7)

To be able to apply the statistical mechanics techniques to the above generalization of the Lotka–Volterra system with account of the spatial dependence, we transform Eqs. (2.2.6) and (2.2.7) to Hamiltonian form. Make the change of variables $q = \ln \phi$, $p = \ln \psi$.

In the new variables, Eqs. (2.2.6) and (2.2.7) take the form

$$\frac{dq}{dt} = 1 - e^p - e^p p_{xx} - e^p (p_x)^2 - e^p p_{yy} - e^p (p_y)^2 .$$  \hspace{1cm} (2.2.8)

$$\frac{dp}{dt} = -1 + e^q + e^q q_{xx} + e^q (q_x)^2 + e^q q_{yy} + e^q (q_y)^2 .$$  \hspace{1cm} (2.2.9)

We reduce the terms containing spatial derivatives appearing in Eqs. (2.2.8) and (2.2.9) to Hamiltonian form. We assume that the values of the spatial derivatives are small and, therefore, we can neglect the quadratic terms. In addition, the same assumptions imply that the coefficients multiplying $e^p$ and $e^q$ may be replaced by constants. Using appropriate linear transformations of the variables $x$ and $y$,
we can make these constants equal to unity. Then, Eqs. (2.2.8) and (2.2.9) take the form

\[ \frac{dq}{dt} = 1 - e^p - p_{xx} - p_{yy}, \tag{2.2.10} \]

\[ \frac{dp}{dt} = -1 + e^q + q_{xx} + q_{yy}. \tag{2.2.11} \]

Equations (2.2.10) and (2.2.11) are Hamiltonian equations with the Hamiltonian

\[ H = \int dx dy (e^q - q + e^p - p + \frac{1}{2} p_x^2 + \frac{1}{2} p_y^2 + \frac{1}{2} q_x^2 + \frac{1}{2} q_y^2). \tag{2.2.12} \]

Unfortunately, the form of Hamiltonian (2.2.12) does not allow one to use Kerner's approach because the statistical sum cannot be explicitly calculated in terms of the gamma functions accurate to elementary functions. To resolve this problem, we select new interaction terms that are similar to the interaction terms in Hamiltonian (2.2.12). These new interaction terms should enable us to calculate the statistical sum in terms of the gamma and elementary functions. We select a replacement for the terms \( p_x^2 \) and \( p_y^2 \) in Hamiltonian (2.2.12) using linear and exponential functions. An appropriate function to replace \( x^2 \) is \( e^x - x \). Instead of the variable \( x \), we will use \( p_x \) and \( p_y \).

Upon the transformations, Hamiltonian (2.2.12) takes the form

\[ H = \int dx dy (e^p - p + e^{p_x} + e^{p_y} - p_x - p_y + e^q - q + e^{q_x} + e^{q_y} - q_x - q_y). \tag{2.2.13} \]

After the integration, the total derivatives \( p_x, p_y, q_x, \) and \( q_y \) disappear. The resulting expression for the Hamiltonian is

\[ H = \int dx dy (e^p - p + e^{p_x} + e^{p_y} + e^q - q + e^{q_x} + e^{q_y}). \tag{2.2.14} \]

For this Hamiltonian, the Hamiltonian equations take the form

\[ \frac{dq}{dt} = 1 - e^p - e^{p_x} p_{xx} - e^{p_y} p_{yy}, \tag{2.2.15} \]

\[ \frac{dp}{dt} = -1 + e^q + e^{q_x} q_{xx} + e^{q_y} q_{yy}. \tag{2.2.16} \]
Due to the above assumption that $p_x$, $p_y$, $q_x$, and $q_y$ are small, the quantities $e^{p_x}$, $e^{p_y}$, $e^{q_x}$, and $e^{q_y}$ are close to unity. The Hamiltonian equations (2.2.15) and (2.2.16) are close to the Hamiltonian equations (2.2.10), (2.2.11). This confirms the fortunate selection of the new spatial terms. In the next section, we calculate the statistical sum for Hamiltonian (2.2.14).

3. Calculation of the Statistical Sum for the Model under Examination

In this section, we calculate the statistical sum for Hamiltonian (2.2.14) with the new spatial terms. To this end, we replace the continuum of the points $x, y$ with the discrete set of points on which the periodic boundary conditions are given. It suffices to select three points on each axis $x$ and $y$. As a result, a square grid consisting of nine points will be used for the calculations. The derivatives of the dependent variables $p$ and $q$ with respect to $x$ and $y$ will be replaced by finite differences. For simplicity, the grid size is set to unity. For convenience, we rename $q$ to $\phi$ and $p$ to $\psi$. Note that, due to the additivity of Hamiltonian (2.2.14), the statistical sum to be calculated is represented as the product of two identical statistical sums

$$Z = Z_1 Z_2 .$$

The statistical sum $Z_1$ has the form

$$Z_1 = \frac{\sum (e^{\phi_{i,j}} - e^{\phi_{i-1,j}})}{e^{-\beta \sum e^{\phi_{i,j}} + e^{\phi_{i-1,j}}}} .$$

The statistical sum $Z_2$ has the same form as $Z_1$.

Following Kerner's method, we try to represent the expression for the statistical sum by a combination of the gamma and elementary functions. However, the term in (3.2) containing $e^{(\phi_{i,j} - \phi_{i-1,j})}$ prevents the representation of the integral of interest as Euler's integral, which is the integral expression for the gamma function. To overcome this difficulty, we make the following transformations in the expression

$$E = e^{-\beta \sum (e^{\phi_{i,j}} - e^{\phi_{i-1,j}})(e^{\phi_{i,j}} - e^{-\phi_{i,j}})}$$

in (3.2). Assume that the major contribution to the statistical sum is made by the small values $\phi_{i,j}$. Then, we have the following heuristic consideration for the transformation of $e^{\phi_{i,j} - \phi_{i-1,j}}$. Note that both $e^{\phi_{i,j}} - 1$ and $e^{-\phi_{i-1,j}} - 1$ are small. Therefore, it holds that
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\[ e^{\phi_{i,j}-\phi_{-i,j}} = e^{\phi_{i,j}} e^{-\phi_{-i,j}} = [1 + (e^{\phi_{i,j}} - 1)][1 + (e^{-\phi_{-i,j}} - 1)] \approx 1 + (e^{\phi_{i,j}} - 1) + (e^{-\phi_{-i,j}} - 1) + \ldots. \]  

(3.4)

Next, we replace \( \phi_{i,j} \) by \( e^{\phi_{i,j}} - 1 \) to obtain

\[ e^{\phi_{i,j} - \phi_{-i,j}} \to e^{\phi_{i,j}} + e^{-(e^{\phi_{-i,j}} - 1)} = e^{\phi_{i,j}} + e^{e^{\phi_{-i,j}}}. \]  

(3.5)

Then, formula (3.3) can be replaced by

\[ e^{-\beta \sum_{i} e^{\phi_{i,j} - \phi_{-i,j}} + (e^{\phi_{i,j} - \phi_{-i,j}}) - \beta \sum_{i} 2 e^{\phi_{i,j}} - \beta \sum_{i} 2 e^{\phi_{-i,j}}} \to e^{-\beta \sum_{i} 2 e^{\phi_{i,j}} - \beta \sum_{i} 2 e^{\phi_{-i,j}}}. \]  

(3.6)

Upon these transformations, the expression for the statistical sum \( Z_1 \) takes the form

\[ Z_1 = \int [d\phi] e^{\sum_{i,j} (\phi_{i,j} - \phi_{-i,j}) - 2\beta \sum_{i} e^{\phi_{i,j}} - 2\beta \sum_{i} e^{\phi_{-i,j}} - (2e\beta) \sum_{i,j} e^{\phi_{i,j}} + (2e\beta)^2 \sum_{k,e} e^{\phi_{i,j}} (\sum_{k,e} e^{\phi_{i,j}}) - \frac{(2e\beta)^3}{6} (\sum_{i,j} e^{\phi_{i,j}})(\sum_{k,e} e^{\phi_{i,j}})(\sum_{p,q} e^{\phi_{i,j}}) + \ldots). \]  

(3.7)

The last term in the exponent in (3.7) prevents one from representing integral (3.7) by Euler's integrals. To overcome this difficulty, we expand the last exponential function in this formula in Taylor's series:

\[ Z_1 = \int [d\phi] e^{\sum_{i,j} (\phi_{i,j} - \phi_{-i,j}) - 2\beta \sum_{i} e^{\phi_{i,j}} - 2\beta \sum_{i} e^{\phi_{-i,j}} - (2e\beta) \sum_{i,j} e^{\phi_{i,j}} + (2e\beta)^2 \sum_{k,e} e^{\phi_{i,j}} (\sum_{k,e} e^{\phi_{i,j}}) - \frac{(2e\beta)^3}{6} (\sum_{i,j} e^{\phi_{i,j}})(\sum_{k,e} e^{\phi_{i,j}})(\sum_{p,q} e^{\phi_{i,j}}) + \ldots). \]  

(3.8)

Now, each term in Taylor's series can be represented by Euler's integral, which has the form

\[ \Gamma(z) = \int_0^\infty t^{z-1} e^{-t} dt. \]  

(3.9)

The typical integral in the series is

\[ I = \int d\phi e^{A\phi - Be^\phi}. \]  

(3.10)

It is reduced to Euler's integral by the change of variables \( t = Be^\phi \):
Thus, we can reduce the series to a combination of the gamma and elementary functions:

$$Z_1 = \left[ \frac{\Gamma(e\beta)}{(e + 2\beta)^{\varphi\theta}} \right]^1 - \frac{(2e\beta)9\Gamma(e\beta)}{(e + 2\beta + 1)^{\varphi\theta}} \left[ \frac{\Gamma(e\beta)}{(e + 2\beta)^{\varphi\theta}} \right]^1 + \frac{(e\beta)2 \Gamma(e\beta)}{2 (e + 2\beta)^{\varphi\theta}} \left[ \frac{9 \Gamma(e\beta)}{(e + 2\beta + 2)^{\varphi\theta}} \right]^1 +$$

$$+ 72 \left[ \frac{\Gamma(e\beta)}{(e + 2\beta + 1)^{\varphi\theta}} \right]^1 - \frac{(2e\beta)^3}{6 \Gamma(e\beta) \left[ \frac{9 \Gamma(e\beta)}{(e + 2\beta + 3)^{\varphi\theta}} \right]^1} +$$

$$+ 81 \left[ \frac{\Gamma(e\beta)}{(e + 2\beta + 2)^{\varphi\theta}} \right]^1 - \frac{9 \Gamma(e\beta)}{(e + 2\beta + 1)^{\varphi\theta}} \left[ \frac{(e\beta)2 \Gamma(e\beta)}{(e + 2\beta)^{\varphi\theta}} \right]^1 + 639 \left[ \frac{\Gamma(e\beta)}{(e + 2\beta + 3)^{\varphi\theta}} \right]^1 + \ldots.$$  

(3.12)

In series (3.12), the combination of the gamma and elementary functions \( \left[ \frac{\Gamma(e\beta)}{(e + 2\beta)^{\varphi\theta}} \right]^1 \) can be factored out, and the remaining terms are represented by elementary functions:

$$Z_1 = \left[ \frac{\Gamma(e\beta)}{(e + 2\beta)^{\varphi\theta}} \right]^1 (1 - (2e\beta)9(1 + \frac{1}{(e + 2\beta)^{\varphi\theta}}) + \frac{(e\beta)2}{2 (1 + \frac{1}{(e + 2\beta)^{\varphi\theta}}) \left[ \frac{9 \Gamma(e\beta)}{(e + 2\beta + 2)^{\varphi\theta}} \right]^1} -$$

$$- \frac{(2e\beta)^3}{6 (1 + \frac{3}{(e + 2\beta)^{\varphi\theta}})} + \frac{81}{(1 + \frac{2}{(e + 2\beta)^{\varphi\theta}}) (1 + \frac{1}{(e + 2\beta)^{\varphi\theta}})^{\varphi\theta}} + \frac{639}{(1 + \frac{1}{(e + 2\beta)^{\varphi\theta}})^{\varphi\theta}}) + \ldots).$$  

(3.13)

It is seen from (3.13) that all terms of the series consisting of elementary functions include the same expression \( 1 + \left( \frac{n}{(e + 2\beta)^{\varphi\theta}} \right) \). For the case \( \beta = 0 \), it is equal to unity:

$$\left(1 + \left( \frac{n}{(e + 2\beta)^{\varphi\theta}} \right) \right)^{\varphi\theta} \bigg|_{\beta=0} = 1.$$  

(3.14)

A remarkable property of this expression is that it tends to a constant as \( \beta \to \infty \). This constant is

$$\left(1 + \left( \frac{n}{(e + 2\beta)^{\varphi\theta}} \right) \right)^{\varphi\theta} \bigg|_{\beta=\infty} = e^{\frac{n\epsilon}{2}}.$$  

(3.15)
Only the linear (in $\beta$) term in (3.13) contains a single expression 

$$1 + \left(\frac{1}{(\varepsilon + 2)\beta}\right)^{\alpha}.$$ 

The coefficients of the other terms with each power of $\beta$ consist of combinations of one or several such expressions. However, the structure of the right-hand side of formula (3.15) is such that all the combinations of exponential functions multiplying $\beta \to \infty$ have the same exponent for each term of the series, which coincides with the index of the series term. This allows us to individually sum up the terms in (3.13) as $\beta \to 0$ and $\beta \to \infty$ and extrapolate the statistical sum using two values of the series. There is a more rigorous approach. The major contribution to the terms of series (3.13) is made by the powers of the function 

$$\left(\frac{1}{1 + (\varepsilon + 2)\beta}\right)^{\alpha}.$$ 

The other terms exhibit similar behavior for each $n$. For this reason, we expand the function 

$$\left(\frac{1}{1 + (\varepsilon + 2)\beta}\right)^{\alpha}$$ 

and its powers into the sum of expressions for each of which series (3.13) can be summed separately. The desired formula has the form

$$\left(\frac{1}{1 + (\varepsilon + 2)\beta}\right)^{\alpha} = e^{-\pi_1\beta} + (1 - e^{-\pi_1\beta})e^{-\frac{n\varepsilon}{e^\varepsilon + 2}}. \quad (3.16)$$

In (3.16), we need to determine the parameters $\alpha_n$. Note that the right-hand side of (3.16) provides the correct value for the power $n$ of the function 

$$\left(\frac{1}{1 + (\varepsilon + 2)\beta}\right)^{\alpha}$$ 

as $\beta \to 0$ and $\beta \to \infty$.

It remains to require the left- and right-hand sides of formula (3.16) be equal at a certain intermediate value of $\beta$. Set $\beta = 1$, and consider the case when $\varepsilon = 1$. Then, the left-hand side of (3.16) is

$$\left(\frac{1}{1 + (\varepsilon + 2)\beta}\right)^{\alpha} \to \left(\frac{3}{4}\right)^n. \quad (3.17)$$

Upon our transformations, formula (3.16) has the form

$$\left(\frac{3}{4}\right)^n = e^{-\pi_1\beta} + (1 - e^{-\pi_1\beta})e^{-\frac{n\varepsilon}{e^\varepsilon + 2}}. \quad (3.18)$$
Now, (3.18) implies a formula for $\overline{a}_n$:
\[
e^{-\overline{a}_n} = \left(\frac{3}{4}\right)^n (e^{-\frac{1}{3}})^n = (0.75)^n - (0.716)^n = (0.75)^n \frac{1 - (0.716)^n}{1 - (0.716)^n} = (0.75)^n \frac{1 - (0.954^n)}{1 - (0.716^n)}.
\]
(3.19)

We transform (3.19) to a form that can be used for the summation of series (3.13):
\[
e^{-\overline{a}_n} = (0.75)^n \frac{1 - (1 - 0.046^n)}{1 - (1 - 0.284^n)} = (0.75)^n \frac{0.046n}{0.284n} = (0.75)^n 0.161.
\]
(3.20)

Formula (3.20) gives the final expression for $\overline{a}_n$. Now we turn to determining the parameter $e^{-\overline{a}_n}$. To this end, we raise the left- and right-hand sides of Eq. (3.20) to the power $\beta$ and introduce the parameters $\gamma_1 = -\ln(0.161)$ and $\alpha_1 = -\ln(0.75)$. Then we obtain
\[
e^{-\overline{a}_n} \beta = e^{\gamma_1 \beta} e^{-n \alpha_1 \beta}.
\]
(3.21)

After these transformations, we can write series (3.13) as
\[
Z_1 = \frac{\Gamma(e\beta)}{(3\beta)^n (e\beta)^n)} (1 - (18e\beta)(e^{-\alpha_1 - \beta_1} + (1 - e^{-\alpha_1 - \beta_1})e^{-\frac{1}{3}}) + \frac{(18e\beta)^2}{2} (e^{-2\alpha_1 - \gamma_1 \beta} + (1 - e^{-2\alpha_1 - \gamma_1 \beta})e^{-\frac{2}{3}}) - \frac{(18e\beta)^3}{6} (e^{-3\alpha_1 - \gamma_1 \beta} + (1 - e^{-3\alpha_1 - \gamma_1 \beta})e^{-1}) + ...\).
\]
(3.22)

Series (3.22) can be divided into three series of which each is just a series for the exponential function with the corresponding exponent. The first series corresponds to $e^{-\gamma_1 \beta} e^{-n \alpha_1 \beta}$, the second series to $e^{-\frac{\alpha_1}{3}}$, and the third series to $e^{-\frac{\alpha_1}{3}} e^{-\gamma_1 \beta} e^{-n \alpha_1 \beta}$. Each of these series is easily summed, which yields the formula
\[
Z_1 = \frac{\Gamma(\beta)}{(3\beta)^n (e\beta)^n)} (1 - (e^{-\gamma_1 \beta} + e^{-\gamma_1 \beta} e^{-18\epsilon \nu e^{-\gamma_1 \beta}} + e^{-18\epsilon \nu e^{-1\gamma_1 \beta}} + e^{-\frac{\alpha_1}{3} - 1 - e^{-\gamma_1 \beta} e^{-18\epsilon \nu e^{-1\gamma_1 \beta}}}) =
= \frac{\Gamma(\beta)}{(3\beta)^n (e\beta)^n)} (e^{-\gamma_1 \beta} e^{-18\epsilon \nu e^{-\gamma_1 \beta}} + e^{-18\epsilon \nu e^{-1\gamma_1 \beta}} - e^{-\gamma_1 \beta} e^{-18\epsilon \nu e^{-1\gamma_1 \beta}}).
\]
(3.23)
The statistical sum (3.23) interpolates the behavior of series (3.13). This fact can be verified in the following way.

As \( \beta \to 0 \), the second and third terms in (3.23) cancel out, and only the first term remains, which takes the form \( e^{-18e\beta} \).

As \( \beta \to 0 \), the same behavior is exhibited by formula (3.13), which confirms the validity of our approximation.

This completes the calculation of the statistical sum for our model. Formula (3.23) gives an approximation of the statistical sum for the generalized Lotka–Volterra system with spatial terms. The derivation of this formula is an achievement because the calculation of the statistical sum for the majority of models is a very difficult task.

We managed to calculate the statistical sum analytically due to the following trick. The last exponential function in (3.7) was expanded in Taylor's series, and Kerner's change of variables was made in each term of this series. As a result, each term of the series was represented by a combination of the gamma and elementary functions. This allowed us to perform the inverse operation, i.e., sum up the remaining series and represent it as a combination of exponential functions multiplied by a term containing the gamma function. This is an advantage of the proposed method because such a combination is most convenient for the further analysis.

In the next section, we will investigate the phase transition in the model using the expression of the statistical sum obtained above.

4. Investigation of the phase transition in the original model

The existence or nonexistence of phase transitions in the system is determined analogously to the Lee–Yang approach [46], [70] by the position of the zeros of the statistical sum on the complex plane. For the analysis of the position of zeros of the statistical sum, only the expression

\[
e^{-\gamma e\beta} e^{-18e\beta e^{-\alpha\beta}} + e^{-18e^{2/3}\beta} - e^{-\gamma e\beta} e^{-18e^{2/3}\beta e^{-\alpha\beta}}\]

in (3.23) is used because the expression in brackets makes no contribution to the zeros of the statistical sum.

For this expression, a simple computer program for determining the absolute value of this expression was developed. This absolute value was plotted using the program Surfer. Figures 1 and 2 show the level lines of the absolute value, which can be used to visually determine the position of zeros of the statistical sum. For the construction of the level lines, the expression

\[
e^{-\gamma e\beta} e^{-18e\beta e^{-\alpha\beta} + 18e^{2/3}\beta} + 1 - e^{-\gamma e\beta} e^{-18e^{2/3}\beta e^{-\alpha\beta} + 18e^{2/3}\beta}\]

was used, which makes it possible to view the surface structure in the domain of the small terms for (3.23).

It is seen from Fig. 1 that the generalized Lotka–Volterra system with spatial terms has a phase transition. This is seen from the behavior of two zeros of the statistical sum, which are symmetric about the real axis. These two zeros are in the right half-plane of the complex plane near the real axis. The distance from the zeros to the real axis is 0.19. The line passing through these zeros intersects the real axis at the point 0.034.
Figure 1 was constructed for the additional spatial terms \( d(e^{p_x} + e^{p_y}) \) in Hamiltonian (2.2.14) for the coefficient \( d = 1 \). This implies that the phase transition point is 0.034.

To verify this result, the level lines for the same model with the coefficient \( d = 3 \) were constructed (Fig. 2). The zeros for this case are clearly seen; they testify that the phase transition also exists in this case. The distance from two symmetric (about the real axis) zeros from the real axis is small—it is equal to 0.13. The line passing through these zeros intersects the real axis at the point 0.03. This implies that the phase transition point is 0.03.

The third (rightmost) zero in Figs. 1 and 2, which lies on the real axis, has nothing to do with phase transitions. This zero appears due to small errors in the calculation of the approximate statistical sum (3.23) as a result of cancelling out small terms consisting of exponential functions with large negative exponents.

Thus, the data above imply that the proposed generalization of the Lotka–Volterra system with spatially distributed parameters has a phase transition.
5. Conclusions

In statistical physics, there are a lot of techniques for the analysis of phase transitions. For each problem, an appropriate most convenient approach can be found. The Lee–Yang method [46], [70] makes it possible to investigate the phase transitions judging by the position of the zeros of the statistical sum on the complex plane. To apply this method, one must know how to calculate the statistical sum, which is a difficult problem. In this paper, the case when this sum can be calculated was considered. A generalization of the Lotka–Volterra system that takes into account the spatial variables was studied. The Lotka–Volterra system has a specific Hamiltonian that allows one to calculate the statistical sum in terms of gamma and elementary functions. A special choice of the spatial terms...
makes it possible to preserve this property for the generalized system, which was done in the present paper. The addition of spatial dependence of the population of species to the classical Lotka–Volterra system makes it possible to study more complex behavior patterns, including the emergence of phase transitions. The Hamiltonian equations (2.2.15), (2.2.16) for the system under examination are nothing more nor less than nonlinear wave equations that have soliton-like solutions. In this system, as in all systems with phase transitions, there are two counteracting factors. The first factor "wants" to order the system in the form of soliton-like solutions. The second factor, in the form of temperature, strives to destroy the ordering. At a certain relation of these factors, a phase transition occurs.

The proper choice of the functions that take into account the spatial dependence of the population of species and their ultimate critical population made it possible to perform all the calculations analytically. As a result, the position of zeros of the statistical sum on the complex plane was analyzed analytically, and the condition of the occurrence of the phase transition was obtained judging by this position. It seems that the study should be continued to obtain a greater number of zeros using a grid with a greater number of points. Since this considerably complicates the mathematical calculations, this issue is left out of the scope of the present paper.

References


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