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Instantons in Spherical Model Thermodynamics

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The instanton thermodynamics of a spherical model analogous to the soliton thermodynamics of one-dimensional sine-Gordon and φ^4-models is constructed. Decomposition of the system phase volume integral into a sum of contributions corresponding to the thermal fluctuations above the basic and instanton vacua is obtained and all the components of this sum are found. It appears that fluctuations above instanton vacua are Gaussian at all temperature. It is shown that the phase transition temperature in the spherical model can be found from the Kosterlitz–Thouless criterion: in the high-temperature phase the instanton configurations become thermodynamically favorable. The obtained results are exact and are naturally formulated in terms of singularity theory.

KEY WORDS: Spherical model; phase transition; instanton; vanishing cycle; monodromy group; singularity theory.

INTRODUCTION

As shown by Berezinskii[1] and Kosterlitz and Thouless,[2,3] the mechanism of phase transition in a system of two-dimensional rotators on the plane is associated with the appearance of vortices: the appearance of a vortex is thermodynamically favorable when the temperature is above T_C. In one-dimensional models (sine-Gordon, φ^4) the kink is an analog of a vortex. In both cases we are dealing with instantons—translationally noninvariant solutions of the following equation:

$$\delta H/\delta\varphi|_{\varphi=\varphi_k}=0 \tag{1}$$

where H is the Hamiltonian, φ is the order parameter, and the subscript k enumerates solutions of (1) in the order of increasing energy. It is well known that the zero temperature of a phase transition in one-dimensional

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systems is a result of the finite energy of the kink. Moreover, the critical behavior for $T \to 0$ is associated with the presence of kinks.[4,5]

It is widely accepted that the increasing role of instanton configurations when the temperature approaches T_C is a sufficiently general result. In this connection we can mention the dislocation theory of melting[2,6,7] and the "cluster picture" of a displacive phase transition[8,9] in two- and three-dimensional systems. However, these approaches have been developed on the phenomenological level and only qualitatively for $d > 2$. The main difficulty here is, on the one hand, the enormous complexity of the nonlinear problem of the phase transition, and, on the other hand, the absence of adequate mathematical language, a firm analytic foundation which would permit us to formulate accurately the basic concepts (clusters, etc.) and to obtain concrete and positive results. We believe that the Picard–Lefschetz theory[10] represents such a language. We shall demonstrate its usefulness in a phase transition problem, using a spherical model modification as an example.

Several structures of the singularity theory can be associated with instantons. The set of critical values $E_k = H(\varphi_k)$ of the Hamiltonian is an elementary one. At these positions the phase volume integral $I(E)$ and the entropy $S(E)$ defined by

$$I(E) = \exp[S(E)] = \int D\varphi \, \delta[H(\varphi) - E] \tag{2}$$

have singularities (van Hove theorem). The next structures, invariant vanishing cycles, a monodromy group, and others, are related to the properties of the analytic continuation of the integral $I(E)$ in the complex plane. They characterize the topological properties of the Hamiltonian level surface and allow one to define correctly the contributions of $I_k(E)$ to the integral (2), which correspond to fluctuations above the instanton vacua φ_k. The singularity theory permits us to associate such contributions not only with stable solutions of Eq. (1), the Hamiltonian minima, but also with unstable ones, the saddle points. Thus, all instantons are unstable in the spherical model, but they are crucial for its thermodynamics. It appears that in this model the fluctuations above the k-instanton vacuum are organized very simply: they have a Gaussian character, and the associated phase volume is given by

$$I_k(E) = A_k(E - E_k)^{(N-3)/2} \tag{3}$$

It is of interest to note that the coefficient A_k and the phase volume $I_k(E)$ are purely imaginary. This unexpected result is connected with the instanton instability. But, in agreement with the Kosterlitz–Thouless concept, these instanton configurations bring one to the phase transition. They become thermodynamically favorable in the high-temperature phase.

The paper is organized as follows. In Section 1 we describe how the main statements of instanton phenomenology can be formulated in terms of the Picard–Lefschetz theory. In Section 2 a spherical model modification is described and its critical points are found. In Section 3 a monodromy group is found and an expansion of the "real" cycle with respect to the basis of vanishing cycles is obtained. It generates a decomposition of the phase volume (2) into a sum of integrals, which correspond to the basic state and instanton contributions. Evaluation of these integrals is performed in Section 4. The results obtained are used in Section 5, where it is shown that the Kosterlitz–Thouless criterion gives a correct energy value of the spherical model phase transition. In Appendices A and B all degenerate singularities of the spherical model Hamiltonian are described. In Appendix C a monodromy group of the Toda-chain Hamiltonian is presented for comparison.

1. STRUCTURES OF THE PICARD–LEFSCHETZ THEORY AND INSTANTON PHYSICS

In this section it is shown how the concepts of singularity theory appear in instanton physics. We restrict ourselves to a heuristic presentation and do not attempt exact statements, which can be found in ref. (10).

The following notation is often used for the integral (2):

$$\int D\varphi\, \delta[H(\varphi)-E] \equiv \int_{\Delta_R} \omega/dH \tag{4}$$

Here ω is the differential N-form, whose dimension N is equal to the number of degrees of freedom

$$\omega = d\varphi^1 \wedge d\varphi^2 \wedge \cdots \wedge d\varphi^N$$

ω/dH is the so-called Gelfand–Leray $(N-1)$-form based on the form ω and the function $H(\varphi)$, and Δ_R is the $(N-1)$-cycle on the $(N-1)$-dimensional level surface of energy E, coinciding with this surface.

The notation on the right-hand side of (4) is convenient for continuation to the complex space. For this purpose one has to consider variables $\varphi^1, \varphi^2,..., \varphi^N$, E as complex and $H(\varphi)$ as an analytical function of N complex variables. In this case the dimension (real) of the $H^{-1}[E]$ level surface is doubled, while the dimension of the cycle Δ_R and the form ω/dH remain the same. Thus, there is "much free space" on the surface $H^{-1}[E]$ and a set of complex cycles is placed on it apart from the real cycle Δ_R.

Complexification greatly simplifies the classification of the level surface. All regular (i.e., without extremal points) constant-energy surfaces are similar. The topology of the critical surface $H^{-1}[E_k]$ depends on the type of critical points on it. If $H(\varphi)$ is a Morse function, the deformation of the regular surface $H^{-1}[E]$ into the singular one $H^{-1}[E_k]$ leads to degeneration into a point of one cycle Δ_k. For the Morse function

$$H = \sum_{\alpha=1}^{N} (\varphi^\alpha)^2 \tag{5}$$

with a single critical point $\varphi = 0$, such a cycle on a regular surface $H^{-1}[E]$, $E \neq 0$, is represented by the $(N-1)$-dimensional sphere

$$\sum_{\alpha=1}^{N} (\varphi^\alpha)^2 = E, \qquad \arg \varphi^\alpha = (\arg E)/2 \tag{6}$$

For the function $H = x^2 - y^2$ the vanishing cycle on $H^{-1}[E]$ with $E > 0$ is

$$x^2 - y^2 = E, \qquad \operatorname{Im} x = \operatorname{Re} y = 0 \tag{7}$$

If $E \to 0$, spheres (6) and (7) are reduced to a point.

Such "vanishing" cycles form a basis on the regular level surface of the Morse function. The real cycle Δ_R can be decomposed with respect to this basis,

$$\Delta_R = \sum_k C_k \cdot \Delta_k \tag{8}$$

with integer C_k.

We may introduce the basic integrals along the vanishing cycles on the surface $H^{-1}[E]$ as

$$I(E, \Delta_k) = \int_{\Delta_k} \omega/dH \tag{9}$$

which are analogous to (2). Their analytical properties are established by singularity theory: they are analytical on the complex E plane with branching at E_k and their branching is completely described by the monodromy group.[10] The decomposition (8) leads naturally to the decomposition of the phase volume (2),

$$I(E) \equiv I(E, \Delta_R) = \sum_k C_k \cdot I(E, \Delta_k) \tag{10}$$

The basic and instanton states are the critical points of the Hamiltonian. Relation (10) is the exact formulation of the statement about the decomposability of the system phase volume into the contributions of "vicinities of the basic state and instanton configurations." It appears, however, that these contributions $I(E, \Delta_k)$ can be complex and non-single-valued function on E and the critical values are their branching points.

We should emphasize the following. The Picard–Lefschetz theory concerns functions with isolated critical points. As a rule, the instanton solutions do not have this property. Indeed, the Hamiltonian usually is invariant under some continuous symmetry, for instance, translations. Its action on an instanton solution leads to a family of analogous solutions. Therefore, it is not the critical points, but the critical lines or surfaces with dimension not larger than the dimension of the symmetry group that conform to the instantons. This situation cannot be described by the Picard–Lefschetz theory.[10] But it is clear how to modify its basic concepts.

The initial real cycle is invariant under the Hamiltonian symmetry group transformations. Therefore, when constructing the basis, we ought to take into account only the invariant vanishing cycles. The action of the monodromy group also must be limited to the subspace of invariant cycles (it is obvious that monodromy transformations do not remove the cycle from this subspace).

The symmetry of the spherical model leads to two types of degenerate singularities described in Appendices A and B.

2. THE SPHERICAL MODEL AND ITS CRITICAL POINTS

The spherical model was proposed for the description of a ferromagnetic phase transition by Kac in 1947. Its exact solution was obtained in 1952 by Berlin and Kac[11] and now the model has been studied in detail.[12] In this and further sections we, without concerning the well-known results obtained in the spherical model, shall be interested in its instantons and the singularity theory structures associated with them.

The starting point is the following modification of the model:

$$H(\varphi)=\sum_{\mathbf{j}}\left[\frac{a\varphi_{\mathbf{j}}^2}{2}+\frac{c}{2}\sum_{\alpha=1}^{d}(\varphi_{\mathbf{j}+\mathbf{e}_\alpha}-\varphi_{\mathbf{j}})^2\right] + \frac{b}{8N}\left(\sum_{\mathbf{j}}\varphi_{\mathbf{j}}^2\right)^2 \tag{11}$$

where $\varphi_{\mathbf{j}+L\mathbf{e}_\alpha}=\varphi_{\mathbf{j}}$, $a<0$, $b>0$, $c>0$. Here $\mathbf{j}=(j_1,..., j_d)$ is an integer vector of the d-dimensional hypercubic lattice, the vectors $\{\mathbf{e}_\alpha\}_{\alpha=1}^{d}$ form an orthonormal basis, and $\varphi_{\mathbf{j}}$ is a real, continuous order parameter (magnetic moment of the $\mathbf{j}$ site). Periodic boundary conditions are supposed, and the summation is over the N sites of the lattice.

After Fourier transformation, we obtain

$$H(\varphi) = \sum_{\mathbf{p}} \frac{\Omega_{\mathbf{p}} \varphi_{\mathbf{p}} \varphi_{-\mathbf{p}}}{2} + \frac{b}{8N} \left(\sum_{\mathbf{p}} \varphi_{\mathbf{p}} \varphi_{-\mathbf{p}} \right)^2 \tag{12}$$

where $\varphi_{\mathbf{p}} = N^{-1/2} \sum_{\mathbf{j}} \varphi_{\mathbf{j}} \exp(-i\mathbf{pj})$, $\mathbf{p} = (2\pi/L)(l_1,..., l_d)$ is the quasimomentum, and $\Omega_{\mathbf{p}} = a + c \sum_{\alpha=1}^{d} |\exp(i\mathbf{pe}_\alpha) - 1|^2$ are frequencies.

Frequencies which correspond to opposite momenta $\mathbf{p}$ and $-\mathbf{p}$ are, or course, equal to each other. On the other hand, some nonopposite momenta have equal frequencies, too. For instance, $\Omega_{\mathbf{p}} = \Omega_{\mathbf{p}'}$ for $\mathbf{p} = (2\pi i/L, 0,...)$, $\mathbf{p}' = (0, 2\pi i/L, 0,...)$. Such coincidences we shall consider as occasional and remove them by small shift of $\Omega_{\mathbf{p}}: \Omega_{\mathbf{p}} \to \Omega_{\mathbf{p}} + \delta\Omega_{\mathbf{p}}$, where $\delta\Omega_{\mathbf{p}} = \delta\Omega_{-\mathbf{p}}$. So from $\Omega_{\mathbf{p}} = \Omega_{\mathbf{p}'}$ it follows that $\mathbf{p} = \pm\mathbf{p}'$.

After the Hamiltonian complexification, the moments $\varphi_{\mathbf{j}}$ become complex and the complex variables $\varphi_{\mathbf{p}}$ and $\varphi_{-\mathbf{p}}$ become independent.

By differentiation of (12) with respect to $\varphi_{-\mathbf{p}}$ we arrive at the equation

$$\left(\Omega_{\mathbf{p}} + b \sum_{\mathbf{p}'} \frac{\varphi_{\mathbf{p}'} \varphi_{-\mathbf{p}'}}{2N} \right) \varphi_{\mathbf{p}} = 0 \tag{13}$$

defining the critical points. Let us enumerate them.

1. The Morse point $\varphi_+ = 0$ corresponding to the paramagnetic phase with the critical value $E_+ = 0$.

2. Two nondegenerate "ferromagnetic" points φ_-^1 and φ_-^2,

$$(\varphi_-^{1,2})_{\mathbf{p}} = \begin{cases} \pm(-2N\Omega_0/b)^{1/2} & (\mathbf{p} = \mathbf{0}) \\ 0 & (\mathbf{p} \neq \mathbf{0}) \end{cases} \tag{14}$$

with the critical value

$$E_- = -\frac{\Omega_0^2 N}{2b} \tag{15}$$

3. Instanton solutions $\varphi^{\mathbf{p}}$, where $\mathbf{p} \neq \mathbf{0}$,

$$(\varphi^{\mathbf{p}})_{\mathbf{p}'} (\varphi^{\mathbf{p}})_{-\mathbf{p}'} = \begin{cases} -\Omega_{\mathbf{p}} N/b & (\mathbf{p}' = \pm\mathbf{p}) \\ 0 & (\mathbf{p}' \neq \pm\mathbf{p}) \end{cases} \tag{16}$$

or, in the coordinate representation,

$$(\varphi^{\mathbf{p}})_{\mathbf{j}} = (-4\Omega_{\mathbf{p}}/b)^{1/2} \cos(\mathbf{pj} + \alpha) \tag{17}$$

where α is an arbitrary parameter describing the instanton translation. The corresponding energies are equal to

$$E_{\mathrm{p}} = -\frac{\Omega_{\mathrm{p}}^2 N}{2b} \tag{18}$$

The critical values in the E plane are shown in Fig. 1 for $a<0$ and $a>0$. The ordering of the instanton energies corresponds to increasing frequencies $\Omega_0 < \Omega_1 < \cdots < \Omega_k < \Omega_{k+1} < \cdots$. For clarity, the energies are removed from the real axis, which corresponds to the shift of a: $a \to a - i0$.

It is useful to enumerate the Hamiltonian critical points in the real subspace $\mathrm{Im}\,\varphi = 0$. For $a<0$ it is doubly degenerate basic state $\varphi_-^{1,2}$, a "paramagnetic" point $\varphi_+ = 0$, and a set of M instanton solutions corresponding to the negative frequencies Ω_{p}. The energies of these instanton solutions are removed into the lower half-plane in Fig. 1a. Let us note that the minima are the $\varphi_-^{1,2}$ points only and all the rest of the extrema are saddle points.

As mentioned in the previous section, certain types of degenerate singularities become stable if the Hamiltonian is invariant under some group of transformations. Moreover, the symmetry group defines completely the set of nonequivalent stable singularities which can have such a Hamiltonian.[13] So, in analyzing the local structures of some degenerate singularity of $H(\varphi)$ (for instance, the topology of the invariant vanishing cycle), we can do this on the equivalent singularity of some table function with symmetry properties that are the same as those of the initial Hamiltonian.

In our case the Hamiltonian (12) is invariant with respect to transformations

$$\varphi_0 \to -\varphi_0 \tag{19a}$$

$$\varphi_{\mathrm{p}} \to \varphi_{\mathrm{p}} \exp(i\alpha), \qquad \varphi_{-\mathrm{p}} \to \varphi_{-\mathrm{p}} \exp(-i\alpha) \tag{19b}$$

The first degeneracy is the coincidence of the energies of two "ferromagnetic vacua" φ_-^1, φ_-^2 resulting from the $\mathbb{Z}_2$ Hamiltonian symmetry (19a). An equivalent singularity is shown in the $\mathbb{Z}_2$-invariant table function from Appendix A. The S_1-symmetry (19b) of the Hamiltonian (12) leads to

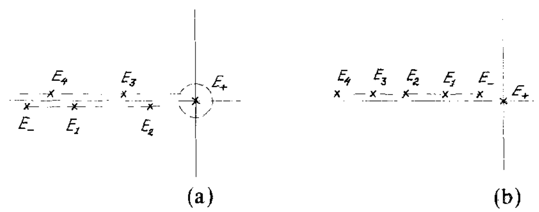


Fig. 1. Critical values of the spherical model (12) for (a) $a<0$ and (b) $a>0$.

the stability of the nonisolated singularity (16): critical points fill the complex curve (16). The S_1-invariant table function from Appendix B has an equivalent singularity in the surface energy E_1.

3. INVARIANT VANISHING CYCLES AND THE MONODROMY GROUP

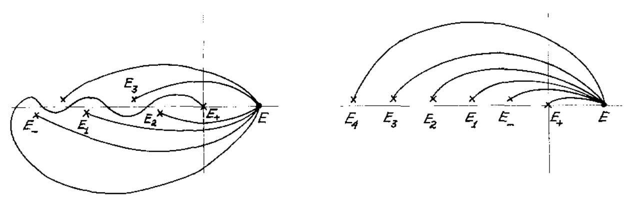
In this section, the bases of invariant [with respect to the symmetry (19)] vanishing cycles are constructed on a regular surface $H^{-1}[E]$, $E>0$ for the Hamiltonian (12) in the cases $a>0$ and $a<0$ and the corresponding representations of the monodromy group are obtained.

An invariant vanishing cycle on the regular surface $H^{-1}[E]$ corresponds to every critical value. An ordinary $(N-1)$-sphere cycle corresponds to the Morse point E_+. On the surface $H^{-1}[E_-]$ the cycle Δ_- vanishes—we have two nonintersecting spheres (see Appendix A). On the surface $H^{-1}[E_k]$ the cycle Δ_k with $S^{N-2}\times S^1$ topology degenerates into a circle (16) (see Appendix B).

Two systems of nonintersecting arcs in the E plane are shown in Fig. 2a and 2b; Fig. 2a refers to the case $a<0$, Fig. 2b corresponds to the case $a>0$. Representations of the monodromy group corresponding to Fig. 2a and 2b are the same and they are described in $N=3(\text{mod } 4)$ by the following relations[2]:

$$\begin{aligned} h_{\gamma_-}(\Delta_-) &= -\Delta_-, & h_{\gamma_-}(\Delta_+) &= \Delta_+ - \Delta_- \\ h_{\gamma_+}(\Delta_-) &= \Delta_- - 2\Delta_+, & h_{\gamma_+}(\Delta_+) &= -\Delta_+ \\ h_{\gamma_k}(\Delta_+) &= \Delta_+ - \Delta_k, & h_{\gamma_k}(\Delta_-) &= \Delta_- - 2\Delta_k \\ & & h_\gamma(\Delta_k) &= \Delta_k \end{aligned} \tag{20}$$

[2] For a cycle Δ which lies on the level surface $H^{-1}[E]$, the homotopy $\Delta(t)$ along the regular curve γ in the E plane $\{\gamma\colon [0,1]\to\mathbb{C},\ \gamma(0)=\gamma(1)=E,\ \gamma(t)\neq E_\alpha\}$ maps Δ onto the starting surface (the cycle $\Delta(t)$ lies on $H^{-1}[\gamma(t)]$). The resulting cycle $\Delta(1)$ may differ from the initial one $\Delta(0)\equiv\Delta$. Thus, one could define an action of the monodromy operator h_γ corresponding to the curve γ: $h_\gamma(\Delta)\equiv\Delta(1)$.



(a) (b)

Fig. 2. Constructing the basis of invariant vanishing cycles for the spherical model for (a) $a<0$ and (b) $a>0$.

where γ is an arbitrary curve with endpoints coinciding at E, and γ_α is an elementary loop[3] associated with the arc u_α. Let us note the trivial action of the monodromy group on the instanton vanishing cycles Δ_k.

When $a<0$ it is useful to have a decomposition of the $\Delta_+(M)$ cycle (M is the number of real instanton solutions φ_k) lying on the $H^{-1}[E]$ surface with possitive E and vanishing at the surface $H^{-1}[0]$ in with real E decreasing to zero. It can be easily obtained using (20) that

$$\Delta_+(M)=h_{\gamma_M}^{-1}\cdot \cdots \cdot h_{\gamma_1}^{-1}\cdot h_{\gamma_-}^{-1}(\Delta_+)=\Delta_+-\Delta_--\sum_{k=1}^{M}\Delta_k \tag{21}$$

The monodromy group is evaluated as follows. Let us observe the movement of critical values in the E plane upon varying a,

$$a(t)=a_0-i\delta-t \tag{22}$$

where $a_0>0$, $t\geqslant 0$, $0<\delta\ll 1$. The point $E_+=0$ is immovable, and all the rest move in the neighborhood of the half straight line $\operatorname{Im} E=0$, $\operatorname{Re} E<0$. They shift to the right, go around zero in the clockwise sense, then move back to the left.[4] In the process of moving, every two critical values become close to each other (they coincide when $\delta=0$) once. The analysis of the appearing degeneracies enables us to reconstruct the whole monodromy group. Let us consider this procedure in more detail. In converting a into zero, the E_- and E_+ critical values merge and the corresponding critical points φ_-^1, φ_-^2, and φ_+ merge, too. For sufficiently small a and E, vanishing cycles Δ_- and Δ_+ can be located in the vicinity of the origin, which enables us to adopt the following approximation:

$$H(\varphi)=\frac{a\varphi_0^2}{2}+\frac{b\varphi_0^4}{8N}+\sum_{\mathbf{p}\neq 0}\frac{\Omega_{\mathbf{p}}\varphi_{\mathbf{p}}\varphi_{-\mathbf{p}}}{2} \tag{23}$$

and to obtain the first four relations in (20), using the results (A.2).

The following degeneracies—coincidence of the critical values E_- and E_1—takes place when $a=a_1$. It is not accompanied by a merging of the corresponding critical points $\varphi_-^{1,2}$ and φ_1 on the surface of the $E_1=E_-$ level. Thus, on the surface $H^{-1}[\tilde{E}]$ neighboring $H^{-1}[E_1]$ and for a values close to a_1, the cycles Δ_1 and Δ_- are far apart and therefore do not "interact" with each other (see Fig. 3a),

$$h_{\gamma_-}(\Delta_1)=\Delta_1, \qquad h_{\tilde{\gamma}_1}(\Delta_-)=\Delta_- \tag{24}$$

[3]An elementary loop γ_α which corresponds to arc u_α is the regular loop (with initial and terminal points coinciding at E) lying in the vicinity of u_α and traversing around the critical value E_α in the counterclockwise sense. In Fig. 7a the elementary loop γ_1^1 corresponds to the arc u_1^1.

[4] Hence, in particular, the equality of two given monodromy group representations yields: deformation (22) continunously transforms Fig. 2b into Fig. 2a.

By transforming them along the arc v in the lower half-plane on the surface of positive energy E, we observe that relations (24) remain valid and for the cycles defined by arcs $\tilde{u}_1$, u_- in Fig. 3b.

A further decrease of the parameter a leads to a nontrivial degeneracy in the conversion into zero of Ω_1 (and hence φ_1 and E_1). For small E_1 and Ω_1 the invariant cycles Δ_1 and $\Delta_+(0)$ (see Fig. 3b) again can be located in the vicinity of zero, which makes the following approximation sufficient:

$$H(\varphi)=\Omega_1\varphi_{\mathbf{p}_1}\varphi_{-\mathbf{p}_1}+\frac{b}{2N}(\varphi_{\mathbf{p}_1}\varphi_{-\mathbf{p}_1})^2+\sum_{\mathbf{p}\neq\mathbf{p}_1}\frac{\Omega_{\mathbf{p}}\varphi_{\mathbf{p}}\varphi_{-\mathbf{p}}}{2} \tag{25}$$

For this Hamiltonian a monodromy group in the basis defined by arcs $u_+(0)$, u_1 in Fig. 3b is described by relations (B.5) of Appendix B. After some algebra, using (A.2) and the identity (see Fig. 3b)

$$\gamma_1\gamma_+(0)=\gamma_+(0)\tilde{\gamma}_1$$

we obtain from (24) and (B.5) all the relations in (20) containing the Δ_1 cycle only (without the rest of the instanton cycles).

By moving a to the left along the real axis and repeating the given analysis for the $\Delta_2, \Delta_3, \ldots, \Delta_k, \ldots$ cycles, we obtain the whole monodromy group (20).

Now let us find the representation of the "real" cycle Δ_R as a linear combination of vanishing cycles. The continuous dependence on energy of the real phase volume (2) provides the following decomposition:

$$\Delta_R=\begin{cases} 0 & (E<E_-) \\ \Delta_- & (E_-<E<E_1) \\ \Delta_-+C_1\Delta_1 & (E_1<E<E_2) \\ \cdots & \cdots \\ \Delta_-+\sum_{k=1}^{M} C_k\Delta_k+C_+\Delta_+(M) & (E>0) \end{cases} \tag{26}$$

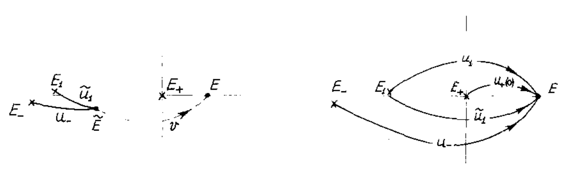


Fig. 3. Cycles Δ_- and $\tilde{\Delta}_1$ do not interact.

where the coefficients C_k and C_+ are integer. Similarly, for $a>0$ we obtain, using the basis shown in Fig. 2b,

$$\Delta_R = \begin{cases} 0 & (E<0) \\ \Delta_+ & (E>0) \end{cases}$$

On the other hand, let us follow the transformation of a real cycle Δ_R on the surface of a fixed positive energy E when a changes along the real axis from a positive value a_0 to a negative value a_1. Note that the surfaces $H^{-1}[E]$ which correspond to the points from the vicinity of the segment (a_0, a_1) are all regular. Thus, an arc joining a_0 with a_1 can be slightly shifted into the $\operatorname{Im} a<0$ half-plane and one may use relation (21). As a result, we obtain that the coefficients C_k and C_+ are all equal to unity:

$$\Delta_R|_{a<0, E>0} = \Delta_+(M) + \Delta_- + \sum_{k=1}^{M} \Delta_k \tag{27}$$

4. EVALUATION OF THE BASIC INTEGRALS

Now let us evaluate, for $E_k<E<E_{k+1}$, the phase volume which corresponds to fluctuations above the kth instanton vacuum:

$$I(E, \Delta_k) = \int_{\Delta_k} \omega/dH \tag{28}$$

The Hamiltonian H is given by (12), and the form ω equals

$$\omega = d\varphi_0 \bigwedge_{k'=1}^{(N-1)/2} (d\varphi_{\mathbf{p}_{k'}} \wedge d\varphi_{-\mathbf{p}_{k'}}/i)$$

One could rewrite the last integral as follows:

$$I(E, \Delta_k) = \kappa(\Delta_k) \int_0^{2\pi} d\alpha \int_{-\infty}^{+\infty} dz \int \prod_{\mathbf{p} \neq \pm \mathbf{p}_k} d\varphi_{\mathbf{p}}\, \delta[H(\varphi, z) - E] \tag{29}$$

where

$$H(\varphi, z) = \sum_{\mathbf{p} \in \pm \mathbf{p}_k} \frac{\omega_{\mathbf{p}} \varphi_{-\mathbf{p}} (\Omega_{\mathbf{p}} - \Omega_k)}{2} + \frac{b}{2N} \left(z + \Omega_k \frac{N}{b} \right)^2 + E_k$$

$$z = \sum_{\mathbf{p}} (\varphi_{\mathbf{p}} \varphi_{-\mathbf{p}}/2), \qquad \alpha = (\log \varphi_{\mathbf{p}_k} - \log \varphi_{-\mathbf{p}_k})/2i$$

$\kappa(\Delta_k)$ is $+1$ or -1 and depends on the orientation of the cycle Δ_k. We integrate over φ_p from $(-i\infty)$ to $(+i\infty)$ if $\Omega_{\mathbf{p}} < \Omega_k$ and from $(-\infty)$ to

$(+\infty)$ if $\Omega_p > \Omega_k$, providing the positive definition of the quadratic form $[H(\varphi, z) - E_k]$. The intersection of the integration volume in (29) with the surface $H^{-1}[E]$ forms a vanishing cycle Δ_k for $E_k < E < E_{k+1}$. An elementary integration yields

$$I(E, \Delta_k) = \pi(2^{N+1}N/b)^{1/2} S_{N-2}(E - E_k)^{(N-3)/2} \times (\Omega_0 - \Omega_k)^{-1/2} \prod_{k' \neq k} (\Omega_{k'} - \Omega_k)^{-1} \tag{30}$$

where S_{N-2} is the surface area of the unit $(N-2)$-sphere. The sign of $I(E, \Delta_k)$ is chosen in such a way that agreement with the decomposition (27) is achieved [see the relation (32) below].

Analytic continuation of (30) to the complex E plane completes the calculation of the instanton integral $I(E, \Delta_k)$. Let us note its basic characteristics.

1. When $E > E_k$ the phase volume integral $I(E, \Delta_k)$ is purely imaginary. This is due to instability of the instanton solutions φ_k which represent saddle points of the Hamiltonian (12).

2. Fluctuations above various instanton vacua do not interact, in the sense that the integral $I(E, \Delta_k)$, being an entire function, is regular at $E_{k'}$ points.

3. The structure of the Hamiltonian $H(\varphi, z)$ in (29) is the same as that of an ensemble of $(N-1)$ uncoupled harmonic oscillators. Hence one can say that fluctuations above every instanton vacuum are Gaussian at all temperatures just as in the ideal gas.

Let us rewrite the above relation as follows:

$$I(E, \Delta) = \int_{C(\Delta)} \frac{d\Omega}{2\pi i} A(\Omega)[E - E(\Omega)]^{(N-3)/2} \tag{31}$$

where

$$A(\Omega) = \pi(2^{N+1}N/b)^{1/2} S_{N-2}(\Omega_0 - \Omega)^{-1/2} \prod_{k'=1}^{(N-1)/2} (\Omega_{k'} - \Omega)^{-1}$$

$E(\Omega) = -N\Omega^2/2b$, and $C(\Delta_k)$ is a small circle around the kth pole of the integrand. Expression (31) also defines integrals $I(E, \Delta_+(M))$, $I(E, \Delta_-)$, and $I(E, \Delta_R)$, provided the integration on the right-hand side is carried out over one of the arcs $C(\Delta_+(M))$, $C(\Delta_-)$, and $C(\Delta_R)$ in the complex Ω plane shown in Fig. 4. From this figure we have

$$I(E, \Delta_R) = I(E, \Delta_-) + \sum_{k=1}^{M} I(E, \Delta_k) + I(E, \Delta_+(M)) \tag{32}$$

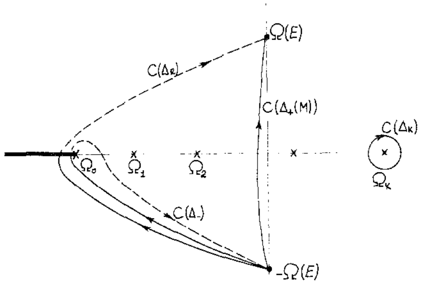


Fig. 4. Integration paths in the Ω plane in (31). Here $\Omega(E) = (-2bE/N)^{1/2}$, $a<0$, and $M=2$.

in agreement with (27). It is not difficult to check that the branching of basic integrals specified by (31) conforms to the monodromy group (20).

Let us note finally that the function $I(E, \Delta_-)$ is analytic in the E plane with exclusion of the real semi-infinite interval $(E_-, +\infty)$. The development is valid when E lies in the indicated interval,

$$\operatorname{Re} I(E, \Delta_-) = I(E, \Delta_R) \tag{33}$$

$$i \operatorname{Im} I(E \pm i0, \Delta_-) = \pm \left[I(E, \Delta_+(M))\, \theta(E) + \sum_{k=1}^{M} I(E, \Delta_k)\, \theta(E - E_k) \right] \tag{34}$$

where

$$\theta(E) = \begin{cases} 1 & (E>0) \\ 0 & (E<0) \end{cases}$$

5. THERMODYNAMIC ASYMPTOTICS AND THE PHASE TRANSITION

It is well known that the thermodynamic asymptotics of the integral (31) can be found by the saddle point method. Figure 5 shows for various energies the dependence of the logarithm of the absolute value of the integrand in (31) on Ω,

$$S(E, \Omega) = \log |A(\Omega)| + \frac{N-3}{2} \log[E - E(\Omega)] \tag{35}$$

All the saddle points $\omega_k(E)$ reside on the real axis and are interlaced with frequencies Ω_k: $\omega_0(E) < \Omega_0 < \omega_1(E) < \Omega_1 < \cdots$. The real phase volume $I(E, \Delta_R)$ is determined by the contribution from the vicinity of the point $\omega_0(E)$.

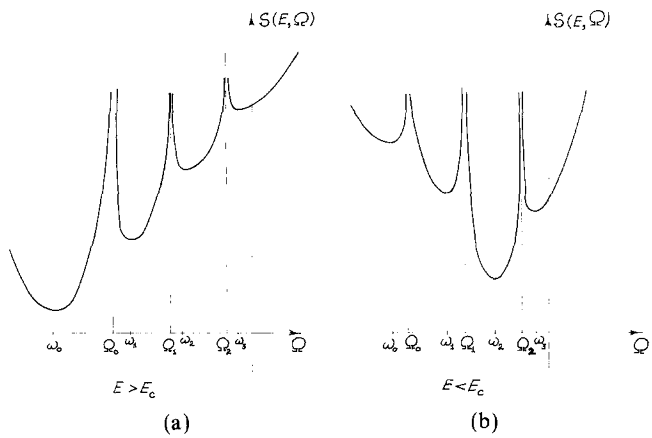


Fig. 5. Dependence of the entropy (35) on Ω in the cases (a) $E > E_C$ and (b) $E < E_C$.

For the energy corresponding to the para phase the lowest saddle [the one with the smallest height $S(E, \omega_0)$] appears at $\omega_0(E)$. With decreasing energy, the point $\omega_0(E)$ moves to the right and at $E = E_C$ a phase transition occurs which results in the tight approach (or sticking, in the thermodynamic limit) of the point $\omega_0(E)$ to the frequency Ω_0.[12] Further decrease of the energy leads to the situation where the point $\omega_1(E)$ becomes a saddle point with the smallest height $S(E, \omega_1)$, then $\omega_2(E)$ (this situation is shown in Fig. 5b), etc. Finally, when $E \to 0$, $\omega_{M+1}(E)$ becomes such a point.

Now let us show that the phase transition being considered is somewhat analogous to the Kosterlitz–Thouless transition. The k number of the instanton solution of the spherical model corresponds to the number of decoupled vortex pairs. The entropy of fluctuations above the kth instanton vacuum at the energy E can be naturally defined as follows:

$$\begin{aligned} S_k(E) &= \log |I(E, \Delta_k)| \\ &\approx \frac{N}{2} \log(E - E_k) - \frac{1}{2} \int \frac{d\mathbf{p}}{(2\pi)^d} \log |\Omega_{\mathbf{p}} - \Omega_k| + \text{const.} \end{aligned} \tag{36}$$

It is obvious that the energy E_C is not a distinguished point for this function, since fluctuations above the kth instanton vacuum "do not feel" the phase transition. However, at the point E_C the relaton between instanton contributions with small k numbers changes (see Figs. 5a and 5b):

$$\left. \frac{\partial S_k(E)}{\partial k} \right|_{k=0} \begin{cases} < 0 & (E < E_C) \\ = 0 & (E = E_C) \\ > 0 & (E > E_C) \end{cases} \tag{37}$$

We can write approximately for the instanton entropy

$$S_k(E) \simeq S(E, \omega_k(E))$$

and point out that for small k the sequence $S(E, \omega_1(E))$, $S(E, \omega_2(E))$,..., $S(E, \omega_k(E))$,... is decreasing or increasing according as the energy E is less or greater than E_c (see Figs. 5a and 5b). One can also arrive at (37) by directly differentiating (36):

$$\left.\frac{\partial S_k(E)}{\partial k}\right|_{k=0} = \left.\frac{\partial \Omega_k}{\partial k}\right|_{k=0} \left\{\frac{N^2\Omega_0}{2b(E-E_0)} + \frac{1}{2}\int \frac{d\mathbf{p}}{(2\pi)^d}(\Omega_{\mathbf{p}} - \Omega_0)^{-1}\right\}$$

The sign of the expression in curly brackets changes at the energy E_c of the phase transition.

The result (37) agrees exactly with the Kosterlitz–Thouless criterion. If $E > E_C$, increasing of k in the vicinity of $k = 0$ (appearance of vortices) increases the system entropy and thus it is thermodynamically favorable.[5] When $E < E_C$ the instanton configurations are thermodynamically not favorable and a ferromagnetic basic state is realized. Ironically, an imaginary phase volume corresponds to instantons. They contribute to the imaginary part of the analytical function $I(E, \Delta_-)$, the real part of which is a real phase volume $I(E, \Delta_R)$ [see (33), (34)].

It is interesting to note that due to the complexification of the Hamiltonian the possibility arises of avoiding the transition into the ferromagnetic phase during the cooling of the system. Indeed, let the (real) system energy decrease from the positive value $E(0)$ to zero,

$$E = E(t) \qquad (0 \leqslant t \leqslant 1)$$

$$E(0) > E_C, \qquad E(1) = 0$$

Here $\omega(t) = \omega_0(E(t))$, which specifies the thermodynamic asymptotics of the real phase volume $I(E(t), \Delta_R)$, moves to the right, approaching the Ω_0 frequency. In order to avoid the approach and merging of the points $\omega(t)$ and Ω_0 (and, hence, the phase transition), let us shift the point $\Omega_0 = \Omega_0(t)$ to the right in the lower half-plane, move it in the clockwise sense around the point $-\Omega(E) = -(-2bE/N)^{1/2}$ [the initial point of the integration contour $C(\Delta_R)$], and then return it to the initial value at a certain value t_1: $\Omega_0(t_1) = a$. Simultaneously, let us continue the decrease of the energy $E(t)$ in such a way that $E(t_1) < E_C$ and during the deformation process the saddle point in $\omega(t)$ is restricted to be the lowest one. As a result, the path

[5] We say the entropy instead of the free energy because we have fixed the energy of the system, but not its temperature.

of integration $C(\Delta(t_1))$ passes between the points Ω_0 and Ω_1. Therefore, the deformation in $0 \leqslant t \leqslant t_1$ yields

$$E(0) \to E(t_1)$$
$$\omega_0(E(0)) \to \omega_1(E(t_1))$$
$$\Delta_R \to \Delta_R - \Delta_-$$
$$C(\Delta_R) \to C(\Delta_R) - C(\Delta_-)$$
$$I(E(0), \Delta_R) \to I(E(t_1), \Delta_R - \Delta_-)$$

where $E(0) > E_C$, $E(t_1) < E_C$. By decreasing the energy to zero for $t = 1$ and avoiding collisions of the saddle point $\omega(t)$ with frequencies $\Omega_1, \Omega_2, ..., \Omega_M$, as was done with Ω_0, we arrive at the desired deformation $\Delta(t)$:

$$\Delta(0) = \Delta_R, \qquad \Delta(t) \underset{t \to 1}{=} \Delta_+(M)$$

and the asymptotics of $I(E(t), \Delta(t))$ over the whole deformation path is defined by the vicinity of the "paramagnetic" point $\omega(t)$ with the smallest height of a saddle.

6. CONCLUSIONS

The main result of the paper is the demonstration of the usefulness of the concepts and methods of complex singularity theory for critical phenomena physics, using the spherical model as an example. The statement about the decomposition of the phase volume into contributions of the basic state and instanton configurations [relations (27), (32)] is formulated most naturally in terms of the Picard–Lefschetz theory. It is shown that fluctuations above instanton vacua do not interact with each other and form an ideal gas. This behavior is closely associated with the trivial action of the monodromy group on the corresponding vanishing cycles. It is also shown that a phase transition takes place in a spherical model in accordance with the Kosterlitz–Thouless criterion: above the temperature of the transition, instanton configurations become thermodynamically favorable.

It will be intriguing to find out which results obtained for the spherical model are applicable to more complex and realistic situations. In this connection, together with the Kosterlith–Thouless criterion, the Gaussian character of fluctuations above the instanton vacuum—one more example of linear behavior in a nonlinear system—is of the greatest interest.

Certainly, this result applies only to the spherical model. Thus, it does not take place in the Toda chain, whose monodromy group is given in Appendix C. Nevertheless, in more complex systems the thermodynamic characteristics corresponding to the fluctuations above the instanton vacuum are perhaps less singular in the vicinity of the phase transition than the corresponding observable quantities.

APPENDIX A

The function

$$H=\frac{ax^2}{2}+\frac{bx^4}{8}+\sum_{n=2}^{N} y_n^2 \tag{A.1}$$

is invariant with respect to the reflection $x\to -x$, which leads to a degenerate singularity. Two critical points lie on the surface of energy $E=-a^2/2b$ and one is located on the surface $H^{-1}[0]$. For $a>0$, $b>0$, the locations of the critical values are shown in Fig. 6a. Two cycles Δ^1_- and Δ^2_- (nonintersecting spheres) vanish on the surface $H^{-1}[E_-]$ and one cycle Δ_+ vanishes on $H^{-1}[0]$. Transforming these cycles along the arcs shown in Fig. 6a, one obtains the basis Δ_+, Δ^1_-, Δ^2_- on the regular surface $H^{-1}[E]$. The monodromy group representation in this basis corresponds to the Dynkin diagram shown in Fig. 6b.[10] Here Δ_+ and $\Delta_-=\Delta^1_-+\Delta^2_-$ are invariant with respect to the reflection cycles. The action of the monodromy group on them in $N=3(\text{mod } 4)$ is described by the relations

$$\begin{aligned} &h_{\gamma_-}(\Delta_-)=-\Delta_-, \qquad && h_{\gamma_-}(\Delta_+)=\Delta_+-\Delta_- \\ &h_{\gamma_+}(\Delta_-)=\Delta_- -2\Delta_+, \qquad && h_{\gamma_+}(\Delta_+)=-\Delta_+ \end{aligned} \tag{A.2}$$

APPENDIX B

The function of the form

$$H=a(x^2+y^2)+\frac{b}{2}(x^2+y^2)^2+\sum_{n=3}^{N} z_n^2 \tag{B.1}$$

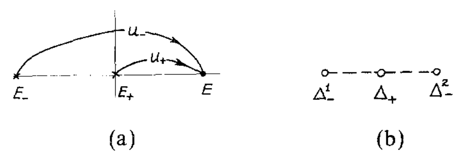


Fig. 6. (a) Constructing the basis of invariant vanishing cycles of $H=\frac{1}{2}ax^2+\frac{1}{8}bx^4+\sum_{n=2}^{N} y_n^2$ for $a>0$ and (b) the corresponding Dynkin diagram.

where $a<0$, $b>0$, and $N=3 \pmod 4$, is invariant with respect to the rotations

$$(x, y, z) \to (x \cos \varphi + y \sin \varphi, \ -x \sin \varphi + y \cos \varphi, z)$$

It has a Morse point at zero with the critical value $E_+ = 0$ and a critical curve $z=0$, $(x^2+y^2) = -a/b$, with the critical value $E_1 = -a^2/2b$. The small deformation

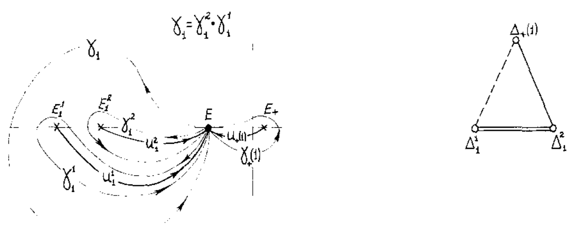
$$H \to \tilde{H} = H - hx$$

with small positive h removes the degeneracy: the critical circle is broken into two Morse points with the energies E_1^1, E_1^2. As a result, we have a Morse function and are under the conditions of the Picard–Lefschetz theory. A basis on the surface $H^{-1}[E]$, $E_1^2 < E < 0$ is formed by the cycles Δ_1^1, Δ_1^2, $\Delta_+(1)$ (notations are the same as in Section 4) vanishing on the surfaces of energies E_1^1, E_1^2, E_+ as the result of deformation along the arcs shown in Fig. 7a. The intersection numbers of these cycles correspond to the Dynkin diagram shown in Fig. 7b. It can be easily found by the methods described in Section 4 of ref. 10, as obtained there in Fig. 32 and 33. In the limit $h \to 0$, the cycles $\Delta_1 = \Delta_1^1 + \Delta_1^2$ and $\Delta_+(1)$ are invariant, which in $E_1 < E < 0$ can be described by the following relations:

$$a(x^2+y^2) + \frac{b}{2}(x^2+y^2)^2 + \sum_{n=3}^{N} z_n^2 = E \tag{B.2}$$

$$\Delta_1: \qquad \operatorname{Im} x = \operatorname{Im} y = \operatorname{Im} z = 0$$

$$\Delta_+(1): \qquad \operatorname{Im} x = \operatorname{Im} y = \operatorname{Re} z = 0$$



(a) (b)

Fig. 7. (a) Constructing the basis of vanishing cycles of the function $H = a(x^2+y^2) + \frac{1}{2}b(x^2+y^2)^2 + \sum_{n=3}^{N} z_n^2 - hx$ on the $H^{-1}[E]$ surface for smul positive h in the case $a<0$, $b>0$. Elementary loops γ_1^1, γ_1^2, and $\gamma_+(1)$ corresponding to arcs u_1^1, u_1^2, and $u_+(1)$ are indicated. (b) The Dynkin diagram of the function under consideration.

The cycle $\Delta_+(1)$ has the topology of a sphere S^{N-1} and for $E \to 0$ it degenerates into a point at the origin. The cycle Δ_1 has the topology of $S^{N-2} \times S^1$ and for $E_0 \to E_1$ it degenerates into a real circle

$$(x^2 + y^2) = -a/b, \qquad \operatorname{Im} x = \operatorname{Im} y = z = 0$$

In the $h \to 0$ limit the points E_1^1 and E_1^2 merge and therefore only two basic loops $\gamma_+(1)$ and $\gamma_1 = \gamma_1^2 \gamma_1^1$ (see Fig. 7a) remain in the E plane. Hence the monodromy group acts on invariant cycles as follows:

$$\begin{aligned} h_{\gamma_1}(\Delta_1) &= \Delta_1, \qquad & h_{\gamma_1}(\Delta_+(1)) &= \Delta_+(1) + \Delta_1 \\ h_{\gamma_+(1)}(\Delta_1) &= \Delta_1, \qquad & h_{\gamma_+(1)}(\Delta_+(1)) &= -\Delta_+(1) \end{aligned} \tag{B.3}$$

where $h_{\gamma_1} = h_{\gamma_1^1} h_{\gamma_1^2}$.

Thus, the monodromy group is trivially acting on Δ_1. This permits us to assume that the corresponding integral $I(E, \Delta_1)$ is analytical at points E_1, E_+. Let us verify this fact. If $a < 0$, $E_1 < E < 0$, we have

$$\begin{aligned} I(E, \Delta_1) &= \int_{\Delta_1} \omega/dH = \int_{-\infty}^{+\infty} dx\, dy \prod_{n=3}^{N} dz_n\, \delta[H(x, y, z) - E] \\ &= \int_{-\infty}^{\infty} \pi\, dt \int_{-\infty}^{+\infty} \prod_{n=3}^{N} dz_n\, \delta\left(at + \frac{bt^2}{2} + \sum_{n=3}^{N} z_n^2 - E\right) \\ &= \pi \int_{-\infty}^{+\infty} d\,\delta t \int_{-\infty}^{+\infty} \prod_{n=3}^{N} dz_n\, \delta\left[\frac{b}{2}(\delta t)^2 + \sum_{n=3}^{N} z_n^2 - \frac{a^2}{2b} - E\right] \\ &= (2/b)^{1/2} \pi S_{N-2} (E - E_1)^{(N-3)/2} \end{aligned} \tag{B.4}$$

where $\delta t = t + a/b$. By analytic continuation of (B.4) to the whole complex plane E we obtain, in accordance with (B.3), a single-valued analytical function.

From (B.3) by continuous deformation and changing the basis, one can derive the monodromy group representation relating to the case of $a > 0$, which is useful in Section 3. This representation corresponds to the

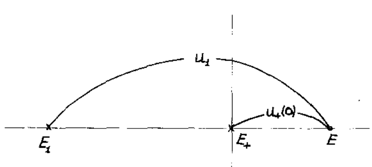


Fig. 8. Constructing the basis of invariant vanishing cycles of $H = a(x^2 + y^2) + \frac{1}{2}b(x^2 + y^2)^2 + \sum_{n=3}^{N} z_n^2$ for $a > 0$.

arcs $u_+(0)$ and u_1 shown in Fig. 8 and is described by the following relations, which are analogous to (B.3):

$$\begin{aligned} h_{\gamma_1}(\Delta_1) &= \Delta_1, \qquad h_{\gamma_1}(\Delta_+(0)) = \Delta_+(0) + \Delta_1 \\ h_{\gamma_+(0)}(\Delta_1) &= \Delta_1, \qquad h_{\gamma_+(0)}(\Delta_+(0)) = -\Delta_+(0) \end{aligned} \tag{B.5}$$

APPENDIX C

In this Appendix we present the monodromy group of the one-dimensional closed Toda chain. Its Hamiltonian has the form

$$H(x_1,..., x_N, y_1,..., y_M) = \sum_{n=1}^{N} \exp(x_n) + \sum_{m=1}^{M} y_m^2 \tag{C.1}$$

with the restriction

$$\sum_{n=1}^{N} x_n = L$$

Here x_n is the distance between neighboring chain atoms, and L is the chain length.

The critical values E_k of the Hamiltonian (C.1) are given by

$$E_k = N \exp[(L - 2\pi ik)/N]$$

where $k = 1,..., N$. Every critical surface $H^{-1}[E_k]$ contains an infinite set of critical points which are nondegenerate. The coordinates of two points x and x' from such a set are connected by the simple relation

$$x'_n - x_n = 2\pi i l_n$$

where $\sum_{n=1}^{N} l_n = 0$, and l_n are integers. We will not distinguish such points and identify corresponding vanishing cycles.

By joining with straight lines the origin of the E plane with the critical values E_k, we obtain the basis of vanishing cycles $\Delta_1, \Delta_2,..., \Delta_N$ on $H^{-1}[0]$. For even M and $(M+N) = 0 (\mathrm{mod}\ 4)$ a monodromy group representation with respect to this basis is described by

$$h_{\gamma_{k'}}(\Delta_k) = \Delta_k + C_{k'k} \Delta_{k'} \tag{C.2}$$

where

$$C_{k'k} = \begin{cases} -2 & (k = k') \\ -\dfrac{N!}{|k-k'|!\,(N-|k-k'|)!} & (k \neq k') \end{cases}$$

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