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Commensurate–Incommensurate Phase Transitions in One-Dimensional Chains

Ya. G. Sinai[1]

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We consider one-dimensional systems of classical particles whose potential energy has the form:

$$W_{\alpha,\gamma} = \sum [\alpha V(x_n) + F(x_n - x_{n-1} | \gamma)]$$

The limit of the Gibbs state as $T \to 0$ is described in terms of invariant measures of two-dimensional mappings which are constructed with the help of $W_{\alpha,\gamma}$. The dependence of these measures on parameters α, γ is investigated.

KEY WORDS: Gibbs state; homoclinic point; invariant pressure.

1. PHASE DIAGRAMS OF ONE-DIMENSIONAL CHAINS AT $T = 0$

We consider a model of one-dimensional interacting particles in an external periodic potential field. A configuration of the minimum energy for the potential of the inner interaction is a lattice whose parameters differ from the parameters of the exterior field. Thus we have a competition of two different tendencies which defines the entire phase picture of the system. One of the main examples is the famous Frenkel–Kontorova model (see Ref. 1) which was introduced in connection with problems of dislocation theory and was discussed from the point of view of epitaxy growth by Frank and Van der Merve.[2] The potential energy of the Frenkel–

[1] L. D. Landau Institute of Theoretical Physics, Academy of Sciences, Moscow V-334, USSR.

Kontorova model has the form

$$W = \alpha \sum_n (1 - \cos 2\pi x_n) + \sum_n (x_n - x_{n-1} - \gamma)^2 \tag{1}$$

We shall deal with a more general case. The potential of the exterior field will be a C^∞-periodic function V of the period 1. We assume that V has nondegenerate minima at the points $x = n$, $-\infty < n < \infty$, and nondegenerate maxima at the points $x = n + \frac{1}{2}$, $-\infty < n < \infty$ and no other critical points. Other "generic" assumptions concerning V will be formulated later. A typical example is $V(x) = \alpha(1 - \cos 2\pi x)$.

The inner interaction between particles acts only between the nearest neighbors. It is defined by a potential energy $F(x - \gamma)$, where F is a C^∞ function, $F(0) = 0$, $F(x) \geqslant 0$, $F''(x) \geqslant c = \text{const} > 0$, and γ is a parameter of the problem. A typical example is $U_a(x) = x^2 + ax^4$. In particular $U_0(x) = x^2$. We shall consider configurations of particles whose potential energy is equal

$$W_{\alpha,\gamma} = \sum_n \left[\alpha V(x_n) + F(x_n - x_{n-1} - \gamma) \right] \tag{1$'$}$$

where α, γ are positive parameters.

The models with the interaction energy (1), (1′) are under discussion in many papers. We can mention the paper by Pokrovsky[3] and its continuation in Ref. 4 and 5, Aubry,[6,7] Bak and von Boehm.[8] In the present paper we shall prove several rigorous results concerning the models (1′). Some of our arguments will be of a purely mathematical character and physicists can omit them without any damage. In such cases we shall write a capital "M" at the beginning and the end of the discussion.

We shall start with the definitions of the configuration space and the limit Gibbs state for the model. A configuration of (1′) is a countable locally finite subset $X \subset R^1$ such that for every $x \in X$ its left and right neighbors x^l, x^r are defined in such a way that (I) $(x^r)^l = x = (x^l)^r$, (II) the graph X with the edges (x, x^r), (x, x^l) is connected, (III) with respect to the natural ordering $x < x^r$ we have $\lim_\uparrow x = \infty$, $\lim_\downarrow x = -\infty$.

Certainly, (I)–(III) do not imply that $x < x^r$ in the sense of the usual ordering on the line. One can say that a configuration of our model is an embedding of the one-dimensional graph with the nearest neighbors into R^1. Certainly it is possible to generalize the situation and to consider embeddings of graphs of a more general structure.

A right (left) semi-infinite tail of a configuration X is a subset $X^r \subset X$ $(X^l \subset X)$ such that if $x \in X^r$ $(x \in X^l)$ then $x^r \in X^r$ $(x^l \in X^l)$ and there exists $x \in X^r$ $(x \in X^l)$ such that $x^l \notin X^r$ $(x^r \notin X^l)$. The space of all configurations X is denoted by M. M. There exists a natural σ-algebra $\mathfrak{S}$ of subsets of M generated by subsets of the following form:

$$A = \Big\{ X \,|\, X \cap \Delta_0 = x \text{ consists of one point, } x^r \in \Delta_1, (x^r)^r \in \Delta_2, \ldots,$$
$$\Big(\underbrace{(x^r)\ldots^r}_{k\text{ times}}\Big) \in \Delta_k, x^l \in \Delta_{-1}, (x^l)^l \in \Delta_{-2}, \ldots,$$
$$\Big(\underbrace{\ldots (x^l)^l \ldots}_{m\text{ times}}\Big)^l \in \Delta_{-m}\Big\}$$

where $\Delta_{-m}, \ldots, \Delta_0, \ldots, \Delta_k$ are Borel subsets of the line.

Denote $M(\Delta_0) = \{X \in M \,|\, \text{card } (X \cap \Delta_0) = 1\}$. We can introduce a partition $\xi^r(\Delta_0)$ $[\xi^l(\Delta_0)]$ of $M(\Delta_0)$ for which an element $C_{\xi^r(\Delta_0)}(C_{\xi^l(\Delta_0)})$ of $\xi^r(\Delta_0)[\xi^l(\Delta_0)]$ is determined by a semiinfinite tail $X^r(X^l)$ whose left (right) end point belongs to Δ_0 and $X \cap \Delta_0$ is exactly this end point. The corresponding σ-algebras $\gamma^{(r)}(\Delta_0), \mathfrak{S}^{(l)}(\Delta_0)$ are generated by subsets

$$A = \Big\{ X \,|\, X \cap \Delta_0' = x \text{ consists of a point,}$$
$$x^r \in \Delta_1, \ldots \Big(\underbrace{\ldots (x^r)^r \ldots}_{k\text{ times}}\Big)^r \in \Delta_k\Big\}$$
$$B = \Big\{ X \,|\, X \cap \Delta_0' = x \text{ consists of a point,}$$
$$x^l \in \Delta_{-1}, \ldots \Big(\underbrace{\ldots (x^l)^l \ldots}_{m\text{ times}}\Big)^l \in \Delta_{-m}\Big\}$$

Here $\Delta_0' \subset \Delta$; $\Delta_1, \ldots, \Delta_k, \Delta_{-1}, \ldots, \Delta_{-m}$ are Borel subsets of the line.

Denote also $M(\Delta_0, \Delta_1) = M(\Delta_0) \cap M(\Delta_1), \mathfrak{S}^{(t)}(\Delta_0, \Delta_1) = \mathfrak{S}^{(l)}(\Delta_0) \vee \mathfrak{S}^{(r)}(\Delta_1)$. We shall define probability distributions on $\mathfrak{S}$. Firstly we want to make more precise the notion of weak convergence of such distributions. Let $\{P_n\}_1^\infty$, P be probability distributions on $\mathfrak{S}$. Assume that $f(x_0, x_1, \ldots, x_k)$ is a continuous function on R^{k+1} with a compact support equal to zero for $x_0 \notin \Delta_0$ where $\Delta_0 \subset R^1$ is an open compact subset. We shall say that P_n converge weakly to P if for any f and $x_0 = X \cap \Delta_0$

$$\lim_{n\to\infty} \int_{M(\Delta_0)} f\Big(x_0, x_0^r, (x_0^r)^r, \ldots, \Big(\underbrace{\ldots (x_0^r)^r \ldots}_{k\text{ times}}\Big)^r\Big)\, dP_n(X)$$
$$= \int_{M(\Delta_0)} f\Big(x_0, x_0^r, (x_0^r)^r, \ldots, \Big(\ldots (x_0^r)^r \ldots\Big)^r\Big)\, dP(X)\mathrm{M}.$$

Now we intend to define limit Gibbs states for models (1′). Let us choose two subsets $\Delta_0, \Delta_1 \subset \mathrm{R}^1$, $\Delta_0 \cap \Delta_1 = \emptyset$ and fix semiinfinite tails X^l, X^r whose end points y^l, y^r belong to Δ_0, Δ_1, respectively. We introduce $M(X^l, X^r) \subset M(\Delta_0, \Delta_1)$ consisting of $X \subset M(\Delta_0, \Delta_1)$ which have X^l, X^r as its tails. It is clear that $M(X^l, X^r) = \cup_{k=0}^{\infty} M_k(X^l, X^r)$, where $M_k(X^l, X^r)$ consists of X for which there are k particles between y^l and y^r in the sense of the graph corresponding to X.

Definition 1. A conditional Gibbs distribution with parameters β and μ under the conditions X^l, X^r is the probability distribution on $M(X^l, X^r)$ such that (I) $P(M_0(X^l, X^r)) = \exp[-\beta F(y^r - y^l - \gamma)]\Xi^{-1}(y^r, y^l;\ \beta, \mu)$ (II) for $k > 0$ its restriction to $M_k(X^l, X^r)$ has the density

$$\Xi^{-1}(y^l, y^r;\ \beta,\ \mu)\exp\left\{-\beta\left[\alpha\sum_{i=1}^{k} V(x_i) + \sum_{i=1}^{k+1} F(x_i - x_{i-1} - \gamma) + \mu k\right]\right\}$$

Here $x_0 = y^l$, $x_{k+1} = y^r$, $x_i = x_{i-1}^r$, and $\Xi(y^l, y^r;\ \beta,\ \mu)$ is the corresponding grand partition function. The integration which is involved in the definition of Ξ is taken over configurations $x_1, \ldots, x_k$ such that $x_i \notin \Delta_0, \Delta_1$, $1 \leqslant i \leqslant k$. Thus Ξ depends also on Δ_0, Δ_1 but we do not denote specially this dependence.

Definition 2. Limit Gibbs state with parameters β and μ is the probability distribution P on $\mathfrak{S}$ such that for every $M(\Delta_0, \Delta_1)$ its restriction to the σ-algebra of subsets of $M(\Delta_0, \Delta_1)$ has the following property: the induced conditional distribution on the σ-subalgebra $\mathfrak{S}^{(t)}(\Delta_0, \Delta_1)$ coincides P a.e. with the conditional Gibbs state in the sense of the definition 1.

As in the case of the usual one-dimensional systems of statistical mechanics the construction and the investigation of limit Gibbs states can be easily done with the help of a version of the transfer matrix. Some results in this direction were obtained in Filonov and Zaslavsky.[9] We shall give an outline of the corresponding arguments. For the simplicity we shall deal with the case $\mu = 0$. Let us consider a cylinder $C = S^1 \times R^1$ with the coordinates (u, z) and introduce the kernel

$$K(u, z \mid u', z') = \delta(u' - (u + z'))$$
$$\times \exp\left\{-\beta\left[\frac{\alpha}{2} V(u) + F(z' - \gamma) + \frac{\alpha}{2} V(u')\right]\right\}$$

We look for a positive eigenfunction of the adjoint operator K^* in the form $g_\beta^*(u', z')\exp[-\beta F(z' - \gamma)]$. Then for g_β^* we get the equation

$$\lambda_\beta g_\beta^*(u', z') = \exp\left\{-\beta\frac{\alpha}{2}\left[V(u' - z') + V(u')\right]\right\}$$
$$\times \int_{-\infty}^{\infty} \exp\left[-\beta F(z - \gamma)\right] g_\beta^*(u' - z', z)\, dz \qquad (2)$$

where λ_β is the corresponding eigenvalue. The solution of (2) belongs to the class of functions periodic with respect to each variable with the period 1. Then (2) can be rewritten as follows:

$$\lambda_\beta g_\beta^*(u',z') = \exp\left\{-\beta\frac{\alpha}{2}\left[V(u'-z')+V(u')\right]\right\} \times \int_0^1 \vartheta_\beta(z-\gamma) g_\beta^*(u'-z',z)\,dz \tag{2'}$$

where $\vartheta_\beta(z) = \sum_{k=-\infty}^{\infty}\exp[-\beta F(z+k)]$.

Also we look for a positive eigenfunction $g_\beta(u)$ of the operator K, i.e.,

$$\lambda_\beta g_\beta(u) = \exp\left[-\beta\frac{\alpha}{2}V(u)\right] \times \int_{-\infty}^{\infty} g_\beta(u+z')\exp\left\{-\beta\left[F(z'-\gamma)+\frac{\alpha}{2}V(u+z')\right]\right\}dz \tag{3}$$

We omit the proof that the solutions of (2′), (3) really exist. These solutions have an important property which is described in the following lemma.

Lemma 1. There exists a positive $C_1 = C_1(\alpha,\gamma)$ for which

$$\exp(-\beta C_1) \leqslant g_\beta^*(u,z),\ g_\beta(u) \leqslant \exp(\beta C_1)$$

Using the function $g_\beta(u)$ we construct a stochastic operator of the transition $(u,z)\to(u',z')$ whose kernel is equal

$$\begin{aligned} Q_\beta(u,z\mid u',z') &= Q_\beta(u\mid u',z') \\ &= \exp\left(-\beta\left\{F(z'-\gamma)+\frac{\alpha}{2}\left[V(u)+V(u')\right]\right\}\right) \\ &\quad\times g_\beta(u')\left[g_\beta(u)\right]^{-1}\lambda_\beta^{-1}\cdot\delta(u'-(u+z')) \end{aligned}$$

The stochastic operator Q defines the Markov chain whose phase space is C. The stationary distribution of the chain has the density $f_\beta(u,z) = g_\beta(u)\cdot g_\beta^*(u,z)\exp[-\beta F(z-\gamma)]$, where the normalization is chosen in such a way that $\int_C f_\beta(u,z)\,du\,dz = 1$.

Assume that $\int z f_\beta(u,z)\,du\,dz > 0$. The connection of the Markov chain with the limit Gibbs state P follows from the fact that the conditional distribution of x^r for fixed $\ldots,(x^l)^l,x^l,x$ is equal to $Q(\{x\}\mid\{x^r\},x^r-x)$, where $\{\cdot\}$ is a fractional part. In other words the conditional distribution of x^r induced by P depends only on $\{x\}$, and in this sense P is a Markov chain. The condition $\int_C z f_\beta(u,z)\,du\,dz > 0$ guarantees that it is concentrated on M.

We shall write $P_{\beta,\alpha,\gamma}$ in order to emphasize the dependence on parameters β,α,γ. The main problem concerns the limit behavior of $P_{\beta,\alpha,\gamma}$ as $\beta\to\infty$. In view of the connection of $P_{\beta,\alpha,\gamma}$ with the Markov chain it is sufficient to investigate the behavior of the Markov chain at $\beta \to \infty$. Let us introduce the space M' of infinite sequences $x' = \{x_i'\}_{-\infty}^{\infty} = \{(u_i, z_i)\}_{-\infty}^{\infty}$, where $x_i' = (u_i, z_i) \in C$. The measure on M' corresponding to the Markov chain is denoted by $P_{\beta,\alpha,\gamma}^{(m)}$. We shall use the following lemma.

Lemma 2. There exists $K = K(\alpha, \gamma) > 0$ such that

$$\lim_{\beta \to \infty} P_{\beta,\alpha,\gamma}^{(m)}(|z_i| > K) = 0 \tag{4}$$

Proof. In view of translation invariance of $P_{\beta,\alpha,\gamma}^{(m)}$ (4) does not depend on i. The density of the stationary distribution has the form $g_\beta(u) g_\beta^*(u,z) \exp[-\beta F(z-\gamma)]$. We shall show that for a $C_2 = C_2(\alpha,\gamma)$,

$$\frac{\max g_\beta(u)}{\min g_\beta(u)}, \frac{\max g_\beta^*(u,z)}{\min g_\beta^*(u,z)} \leqslant \exp(C_2 \beta) \tag{5}$$

from which the statement of lemma easily follows. Let us put

$$g_\beta(u) = \exp\left[-\beta \frac{\alpha}{2} V(u)\right] r_\beta(u).$$

Then

$$\lambda_\beta r_\beta(u) = \int_{S^1} \vartheta_\beta(u - w - \gamma) r_\beta(w) \exp\left[-\frac{\beta\alpha}{2} V(w)\right] dw$$

$$\frac{r_\beta'(u)}{r_\beta(u)}$$

$$= \frac{\int_{S^1} [\vartheta_\beta'(u-w-\gamma)/\vartheta_\beta(u-w-\gamma)] r_\beta(w) \exp[-\beta(\alpha/2)V(w)]\,dw}{\int_{S^1} r_\beta(w) \exp[-\beta(\alpha/2)V(w)]\,dw}$$

We shall use the inequality $|\vartheta_\beta'(w)| \vartheta_\beta^{-1}(w) \leqslant C_3 \beta$ for some $C_3 = C_3(\gamma)$ which can be easily obtained by direct estimations. It gives

$$\max_u \ln r_\beta(u) - \min_u \ln r_\beta(u) \leqslant C_3 \beta$$

Thus we have (5) for $g_\beta(u)$. The proof for $g_\beta^*(u,z)$ goes in a similar way. ■

Now we introduce the transformation T_0 of C onto itself, which plays a crucial role in the further part of the paper. Namely, we put $T_0(u,z) = (u', z')$, where

$$F'(z' - \gamma) = F'(z - \gamma) + \frac{\alpha}{2} V'(u)$$

$$u' = u + z'$$

In view of our conditions concerning F the point (u', z') is defined uniquely.

Let $M'_0 \subset M'$ be the space of trajectories of T_0, i.e., the space of sequences $x' = \{(u_i, z_i)\}_{-\infty}^{\infty}$ such that $(u_{i+1}, z_{i+1}) = T_0(u_i, z_i)$, $-\infty < i < \infty$.

Theorem 1. Let $\Pi_{\alpha,\gamma}$ be a limit point of measures $P^{(m)}_{\beta,\alpha,\gamma}$ in the sense of weak convergence as $\beta \to \infty$. Then $\Pi_{\alpha,\gamma}(M'_0) = 1$.

Remark. In the case of lattice systems of statistical mechanics a similar result is contained in Dobrushin and Pecherski.[10]

Before proving the theorem we derive an important corollary.

Corollary 1. Let μ be a measure on C for which $\mu(A) = \Pi_{\alpha,\gamma}(x' \mid (u_0, z_0) \in A)$, $A \subset C$. Then μ is an invariant measure for T_0.

The statement follows easily from the translation invariance of $\Pi_{\alpha,\gamma}$ and from the definition of the weak convergence.

Proof of Theorem 1. We put

$$\Gamma = \left\{(u_1, z_1), (u_2, z_2) \mid u_2 = u_1 + z_1, F'(z_2 - \gamma) = F'(z_1 - \gamma) + \frac{\alpha}{2} V'(u_1)\right\}$$
$$\in C \times C$$

Let us take a continuous function $\Phi((u_1, z_1), (u_2, z_2))$ with a compact support which is equal to zero in a neighborhood of Γ. We shall show that $\int \Phi \, d\Pi_{\alpha,\gamma} = 0$. We have

$$\int \Phi((u_1, z_1), (u_2, z_2)) \, dP^{(m)}_{\beta,\alpha,\gamma} = \int_{|z_1|, |z_2|, |z_3| \leqslant K} \Phi \, dP^{(m)}_{\beta,\alpha,\gamma} + \mathfrak{I}$$

In view of Lemma 2 $\mathfrak{I} \to 0$ as $\beta \to \infty$. The first integral can be rewritten in the following way:

$$\begin{aligned}
\mathfrak{I}_0 &= \int_{|z_1|, |z_2|, |z_3| \leqslant K} \Phi \, dP^{(m)}_{\beta,\alpha,\gamma} \\
&= \int_{|z_3| \leqslant K} dP^{(m)}_{\beta,\alpha,\gamma} \int \Phi((u_1, z_1), (u_2, z_2)) \, dP^{(m)}_{\beta,\alpha,\gamma} \\
&\qquad \times ((u_1, z_1), (u_2, z_2) \mid (u_0, z_0), (u_3, z_3))
\end{aligned} \tag{6}$$

Let us consider in more detail the conditional distribution which enters in the last integral. It follows from the definition of our Markov chain that it does not depend on z_0 and its dependence on u_3, z_3 follows from the equality $u_0 + z_1 + z_2 \equiv u_3 - z_3 \pmod 1$. This means that $u_0 + z_1 + z_2 = u_3 - z_3 + i$ for some i, $|i| \leqslant 3K$. The conditional distribution has the form

$$\text{const} \exp\{-\beta[F(z_1 - \gamma) + F(z_2 - \gamma) + \alpha V(u_0 + z_1) + \alpha V(u_0 + z_1 + z_2)]\}$$
$$\times \delta(u_3 - z_1 - z_2 - z_3 - u_0)$$

where const is a normalizing factor and δ is the δ-function on S^1.

Put $G(z_1,z_2) = F(z_1-\gamma) + F(z_2-\gamma) + \alpha V(u_0+z_1) + \alpha V(u_0+z_1+z_2)$. Here u_0 is considered as a parameter. Let us find values of z_1, z_2 for which G takes a minimum under the condition $z_1+z_2 = u_3 - z_3 + i$. Denote $G_\lambda(z_1,z_2) = G(z_1,z_2) - \lambda(z_1+z_2)$. Then

$$F'(z_1-\gamma) + \alpha V'(u_0+z_1) + \alpha V'(u_0+z_1+z_2) - \lambda = 0$$
$$F'(z_2-\gamma) + \alpha V'(u_0+z_1z_2) - \lambda = 0$$

which implies $F'(z_2-\gamma) = F'(z_1-\gamma) + \alpha V'(u_0+z_1)$. In other words the minimal points $(u_1,z_1),(u_2,z_2) \in \Gamma$. The first equality can be used for finding of z_1 as a function of λ. Then λ can be found from the equation $z_1+z_2 = u_3 - z_3 - u_0 + i$.

Thus for every condition the minimal value of G is taken on a point of Γ. In view of compactness of the set of conditions in (6) one can find a small neighborhood $O \subset C \times C \backslash \operatorname{supp}\Phi$ of the set Γ that for a $\delta > 0$

$$G(z_1,z_2) \geqslant G_{\min} + \delta, \qquad (u_1,z_1),(u_2,z_2) \in C \times C \backslash O$$

From the other side for a $\rho > 0$ and the ρ-neighborhood O' of the set of all minimal points we have $G(z_1,z_2) \leqslant G_{\min} + (1/2)\delta$, if $((u_1,z_1),(u_2,z_2)) \in O' \subset C \times C$. This easily leads to

$$\int \Phi \, dP^{(m)}_{\beta,\alpha,\gamma}((u_1,z_1),(u_2,z_2) \,|\, (u_0,z_0),(u_3,z_3)) \to O \qquad \text{as} \quad \beta \to \infty$$

uniformly over all conditions. Thus $\mathfrak{I}_0 \to O$ as $\beta \to \infty$. ■

Now we can introduce the main definition.

Definition 3. Phase diagram of the model (1′) is a function $I_{\alpha,\gamma}$ which maps the space of parameters (α,γ) into the set of normed invariant measures of T_0 in view of Corollary 1.

Remark. Certainly one can consider another two-parameter families of interactions. An extension of Definition 3 to such cases is obvious.

Let $\mathfrak{M}$ be the space of normed invariant measures μ of T_0, $H(u,z) = \alpha V(u) + F(z-\gamma)$ and

$$h(\mu) = \int H(u,z)\, d\mu, \qquad \mu \in \mathfrak{M}$$

$h_{\alpha,\gamma} = \min_{\mu \in \mathfrak{M}} h(\mu)$. We recall that $\mathfrak{M}$ is a closed compact set in the weak topology. In the second part of this paper the following theorem plays the crucial role.

Theorem 2. Let $\Pi_{\alpha,\gamma}$ be a limit point of $P^{(m)}_{\beta,\alpha,\gamma}$ as $\beta \to \infty$ and $\mu \in \mathfrak{M}$ is the corresponding measure. Then $h(\mu) = h_{\alpha,\gamma}$.

Before proving the theorem we shall explain how we shall employ it. Suppose that the minimum $h_{\alpha,\gamma}$ is attained on a single measure μ_0. Then it gives immediately $I_{\alpha,\gamma} = \mu_0$.

Proof. Assume that $h(\mu) > h_{\alpha,\gamma}$. Then $\mu = \mu_1 + \mu_2$ where μ_1, μ_2 are mutually singular, $h(\mu_2) = h_{\alpha,\gamma}$, and for μ_1–almost every (u_0, z_0),

$$\lim_{N\to\infty} \frac{1}{N} \sum_{i=0}^{N} H\big(T_0^i(u_0, z_0)\big) > h_{\alpha,\gamma}$$

Certainly it may happen that $\mu_2 = 0$. Take $\epsilon > 0$ and find $\delta > 0$, $N > 0$, for which the set $A \subset C$ of points (u_0, z_0), where

$$\frac{1}{N} \sum_{i=0}^{N} H\big(T_0^i(u_0, z_0)\big) \geqslant h_{\alpha,\gamma} + \delta$$

is such that $\mu_1(A) \geqslant \mu_1(C) - \epsilon$ and the set $B \subset C$ of points (u_0, z_0), where

$$\frac{1}{N} \sum_{i=0}^{N} H\big(T_0^i(u_0, z_0)\big) < h_{\alpha,\gamma} + \frac{1}{4}\delta$$

is such that $\mu_2(B) \geqslant \mu_2(C) - \epsilon$. Let us fix a nonnegative continuous function $\varphi(u_0, z_0)$ which is equal to zero outside A and $\int \varphi \, d\mu_1 > 0$. Now we construct a nonnegative continuous function Φ on $\underbrace{C \times C \times \cdots \times C}_{N+1 \text{ times}}$,

$$\Phi\big((u_0, z_0), T_0(u_0, z_0), \ldots, T_0^N(u_0, z_0)\big) = \varphi(u_0, z_0)$$

and for all $((u_0, z_0), (u_1, z_1), \ldots, (u_N, z_N)) \in \operatorname{supp}\Phi$ we have $(1/N) \sum_{i=0}^{N} H(T_0^i(u_0, z_0)) \geqslant h_{\alpha,\gamma} + (2/3)\delta$. Then for any sequence of $\beta \to \infty$

$$\begin{aligned} &\int \Phi((u_0, z_0), (u_1, z_1), \ldots, (u_N, z_N)) \, dP_{\beta,\alpha,\gamma}^{(m)} \\ &\qquad \to \int \varphi(u_0, z_0) \, d\mu\,((u_0, z_0)) \geqslant \int \varphi(u_0, z_0) \, d\mu_1 > 0 \end{aligned} \tag{7}$$

From the other side we shall show that the integral in (7) tends to zero as $\beta \to \infty$. We have

$$\begin{aligned} &\int \Phi((u_0, z_0), (u_1, z_1), \ldots, (u_N, z_N)) \, dP_{\beta,\alpha,\gamma}^{(m)} \\ &\quad = \int dP_{\beta,\alpha,\gamma}^{(m)} \int \Phi((u_0, z_0), \ldots, (u_N, z_N)) \, dP_{\beta,\alpha,\gamma}^{(m)} \\ &\qquad \times \big((u_0, z_0), \ldots, (u_N, z_N) \,|\, (u_{-1}, z_{-1}), (u_{N+1}, z_{N+1})\big) \end{aligned} \tag{8}$$

As in Theorem 1 we can restrict ourselves by the integration over the set of variables, where $|z_i| \leqslant K$, $O \leqslant i \leqslant N$. Then the inner integral in (7) is not more than const$|\max \Phi| \cdot K^N \cdot \exp\{-\beta[h_{\alpha,\gamma} + (2/3)\delta]N\}$ where const is a normed factor of the conditional distribution. In order to estimate const we remark that one can find a sufficiently small neighborhood O'' of the set

$$\underbrace{\tilde{B} \subset C \times \cdots \times C,}_{(N+1) \text{ times}} \qquad \tilde{B} = \{(u_0, z_0), (u_1, z_1), \ldots, (u_N, z_N)\}, (u_i, z_i)$$
$$= T_0^i(u_0, z_0)$$

and $(u_0, z_0) \in B$ such that

$$\frac{1}{N}\sum_{i=0}^{N} H((u_i, z_i)) \leqslant h_{\alpha,\gamma} + \frac{1}{3}\delta, \qquad ((u_0, z_0), \ldots, (u_N, z_N)) \in O''$$

It follows from the explicit form of the conditional distribution that

$$\begin{aligned} 1 &\geqslant P^{(m)}_{\beta,\alpha,\gamma}\big(\tilde{B}\,|\,(u_{-1}, z_{-1}), (u_{N+1}, z_{N+1})\big) \\ &> \operatorname{const}\operatorname{vol}(O'')\exp\big[-\beta N\big(h_{\alpha,\gamma} + \tfrac{1}{3}\delta\big)\big] \end{aligned}$$

Therefore const $\leqslant [\operatorname{vol}(O'')]^{-1}\exp\{[h_{\alpha,\gamma} + (1/3)\delta]N\}$, and

$$\begin{aligned} &\operatorname{const}\max|\Phi| \cdot K^N \exp\big[-\beta\big(h_{\alpha,\gamma} + \tfrac{2}{3}\delta\big)N\big] \\ &\leqslant \max|\phi| \cdot K^N \cdot (\operatorname{vol}(O''))^{-1} \cdot \exp\Big(-\beta\frac{\delta}{3}N\Big) \to 0 \end{aligned}$$

as $\beta \to \infty$. We conclude that the left-hand part of (8) tends to zero while it must stay positive in view of (7).

2. AN ANALYSIS OF THE PHASE DIAGRAM IN A CONTINUUM LIMIT

In the last two sections we shall consider the case of small α and $F(x) = (1/2)x^2 + \alpha F_1(x/\sqrt{\alpha})$. The second term is considered as a small perturbation of the quadratic potential. We assume that $F_1(0) = 0$, $F_1(x) > 0$ for $x \neq 0$, $F_1'' \geqslant -c > -1$ for some $c > 0$. Let us make the change of variables $z - 1 = \sqrt{\alpha}\, Z$, $u = U$, and put $\gamma - 1 = \sqrt{\alpha}\,\Gamma$. In new variables the transformation T_0 takes the form

$$\begin{aligned} Z' + F_1'(Z' - \Gamma) &= Z + F_1'(Z - \Gamma) + \frac{\sqrt{\alpha}}{2} V'(U) \\ U' &= U + \sqrt{\alpha}\, Z' \qquad (\mathrm{mod}\ 1) \end{aligned} \tag{9}$$

Assume that α is small. Then (9) can be considered as a difference approximation with the time step $\Delta t = \sqrt{\alpha}$ of the system

$$\frac{dU}{dt} = Z, \qquad \frac{dZ}{dt} = \frac{V'(U)}{2 + 2F_1''(Z - \Gamma)} \tag{10}$$

The system (10) has the first integral $\mathcal{H}_0 = -V(U) + Z^2 + 2ZF_1'(Z - \Gamma) - 2F_1(Z - \Gamma)$. The function $G(Z) = Z^2 + 2ZF_1'(Z - \Gamma) - 2F_1(Z - \Gamma)$ is strictly monotone for $Z > 0$, $Z < 0$, because $G'(Z) = 2Z[1 + F_1''(Z - \Gamma)]$. Thus for every constant k the equality $G(Z) = k + V(u)$ defines two curves $Z = \mathfrak{L}_k^{\pm}(u)$. For $k_0 = G(0)$ these curves pass through the fixed point $(0, 0)$ of the system (10) and in fact are its stable and unstable separatrices. For $k < k_0$ the curves $\mathfrak{L}_k^{\pm}(U)$ are two parts of a closed curve $\mathfrak{L}_k(U)$, while for

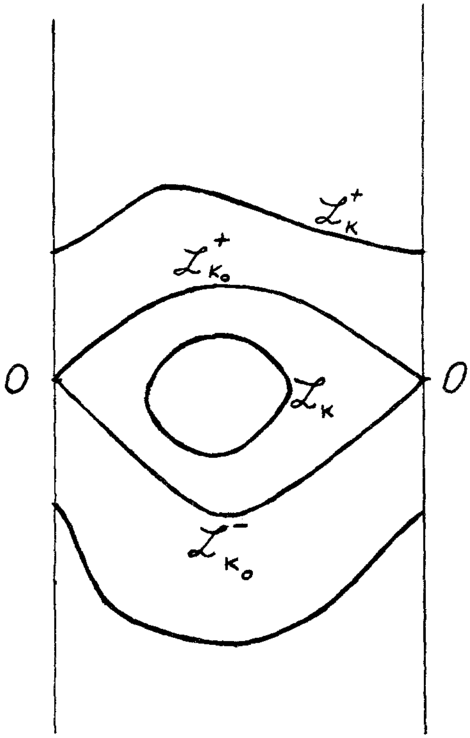


Fig. 1.

$k > k_0$ these curves are different closed curves on the cylinder C. The form of all curves is similar to that one for $F_1 = 0$ and is drawn on Fig. 1.

Ergodic invariant normed measures for the system (10) are concentrated either on $\mathfrak{L}_k^{\pm}$, $k \neq k_0$, or on $\mathfrak{L}_k$, $k < k_0$, or at the point $(0,0)$. We shall denote them by $\mu_{k^\pm}$, μ_k, or $\mu^{(0)}$, respectively.

Let us recall that the energy per particle which enters Theorem 2 has the form $(\alpha/2)V(u) + (z-\gamma)^2/2 + \alpha F_1[(z-\gamma)/\sqrt{\alpha}\,] = \alpha(\frac{1}{2}V(u) + \frac{1}{2}(Z-\Gamma)^2 + F_1(Z-\Gamma))$. We put $H^{(c)}(U,Z) = \frac{1}{2}V(U) + \frac{1}{2}(Z-\Gamma)^2 + F_1(Z-\Gamma)$ and for each invariant normed measure μ of the system (10) $h^{(c)}(\mu) = \int H^{(c)}(U,Z)\,d\mu$. Let be also $h_\Gamma^{(c)} = \min_\mu h^{(c)}(\mu)$. The following definition is an analogy to Definition 3.

Definition 3′. The phase diagram of the system (10) is the function $\mathfrak{T} : \Gamma \to I_\Gamma = \{\, \mu \mid h_\Gamma^{(c)} = h_{(\mu)}^{(c)} \}$.

We shall investigate the phase diagram in more detail. Firstly we consider the case when $F_1 = 0$. Then $h^{(c)}(\mu^{(0)}) = \frac{1}{2}\Gamma^2$ in view of $V(0) = 0$.

For $k < 0$

$$h^{(c)}(\mu_k) - h^{(c)}(\mu^{(0)}) = \int \left[\tfrac{1}{2} V(U) + \tfrac{1}{2} Z^2 - \Gamma Z \right] d\mu_k$$
$$= \int \left[\tfrac{1}{2} V(U) + \tfrac{1}{2} Z^2 \right] d\mu_k > 0$$

because $\int Z\, d\mu_k = 0$ due to $d\mu = T^{-1}(k)\,dt$, where $T(k)$ is the period of motion along $\mathfrak{L}_k$, $Z\,dt = dU$, and $\int_{\mathfrak{L}_k} dU = 0$. Thus $h^{(c)}(\mu_k) - h^{(c)}(\mu^{(0)}) > 0$ for $k < 0$ and such μ_k never belong to the range of $\mathfrak{T}$.

For $k > 0$ it is meaningful by the same reason to consider only the curves $\mathfrak{L}_k^+$. We have again

$$h^{(c)}(\mu_k) - h^{(c)}(\mu^{(0)}) = \int \left[\tfrac{1}{2} V(U) + \tfrac{1}{2} Z^2 \right] d\mu_k - \Gamma \int Z\, d\mu_k$$

and $d\mu_k = T^{-1}(k^+)\,dt = Z^{-1} T^{-1}(k^+)\,dU$. It gives

$$\int Z\, d\mu_k = \frac{1}{T(k^+)} \int Z\, dt = \frac{1}{T(k^+)} \int dU = \frac{1}{T(k^+)} \tag{11}$$

From the equality $Z^2 = k + V(U)$ we get

$$\tfrac{1}{2} \int \left[V(U) + Z^2 \right] d\mu_k = \int Z^2\, d\mu_k - \tfrac{1}{2} k = \left[T(k^+) \right]^{-1} \int Z^2\, dt - \tfrac{1}{2} k$$
$$= \left[T(k^+) \right]^{-1} \int_0^1 Z\, dU - \tfrac{1}{2} k$$
$$= \left[T(k^+) \right]^{-1} \int_0^1 \sqrt{\left[k + V(U) \right]}^{\,1/2} dU - \tfrac{1}{2} k$$

It is easy to see that $T(k^+) = \int_0^1 [k + V(U)]^{-1/2}\, dU$ and

$$h(k) = h^{(c)}(\mu_{k^+}) - h^{(c)}(\mu^{(0)})$$
$$= \left\{ \int_0^1 \sqrt{\left[k + V(U) \right]}^{\,1/2} dU \right\} \left\{ \int_0^1 \left[k + V(U) \right]^{-1/2} dU \right\}^{-1}$$
$$- \tfrac{1}{2} k - \Gamma \left\{ \int_0^1 \left[k + V(U) \right]^{-1/2} dU \right\}^{-1}$$

$$\frac{dh}{dk} = \left\{ \int_0^1 \left[k + V(U) \right]^{1/2} dU - \Gamma \right\} \frac{d}{dk} \left\{ \int_0^1 \left[k + V(U) \right]^{1/2} dU \right\}^{-1}$$

One can easily see that $(d/dk)\{\int_0^1 [k + V(U)]^{-1/2}\, dU\}^{-1} > 0$.

Therefore (1) for $\Gamma \leqslant \Gamma_0 = \int_0^1 \sqrt{[V(U)]}^{\,1/2}\, dU$ the derivative $dh/dk > 0$ for $k > 0$ and $dh/dk|_{k=0} \geqslant 0$, i.e., $\min_{k \geqslant 0} h(k) = h(0) = \lim_{k \to 0} h(k) = 0$.

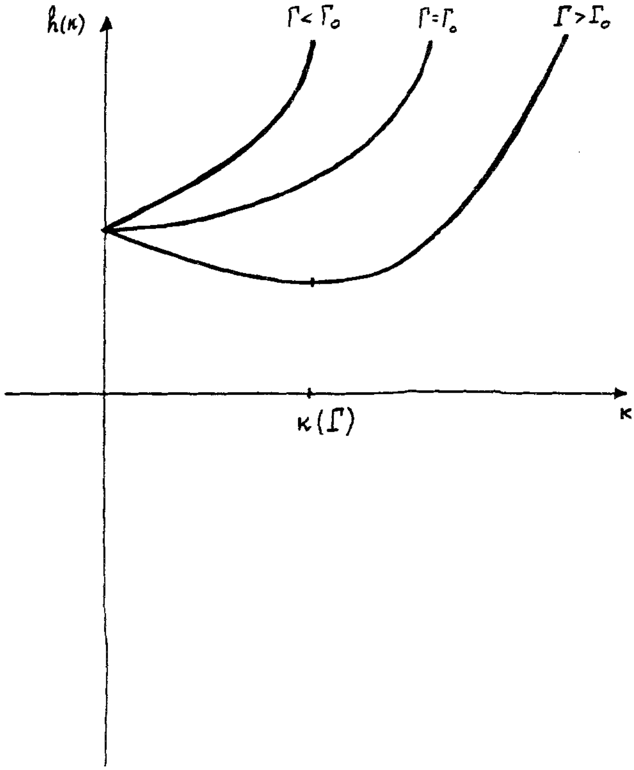


Fig. 2.

(2) For $\Gamma > \Gamma_0$ $\min_{k \geqslant 0} h(k) = h(k(\Gamma))$, where $k(\Gamma)$ is the solution of the equation $\int_0^1 \sqrt{[k + V(U)]}^{1/2}\, dU = \Gamma$. In this case $\mathfrak{T}(\Gamma) = \mu_{k^+(\Gamma)}$.

Different cases are drawn on Fig. 2.

Returning to the case $F_1 \neq 0$ but for F_1 sufficiently small we can formulate the following result.

Theorem 3. Let us fix an interval $[0, \Gamma_1]$ where $\Gamma_1 > \Gamma_0$. One can find $c_1 > 0$ such that if $|F_1(x)|, |(d^i/dx^i)F_1(x)| \leqslant c_1$, $1 \leqslant i \leqslant 3$, then there exist $\overline{\Gamma}_0 = \overline{\Gamma}_0(F_1) \in [0, \Gamma_1]$ for which $\mathfrak{T}(\Gamma) = \mu^{(0)}$ if $0 \leqslant \Gamma \leqslant \overline{\Gamma}_0$ and a continuous increasing function $k = k(\Gamma)$, $\overline{\Gamma}_0 < \Gamma \leqslant \Gamma_1$ such that for these Γ we have $\mathfrak{T}(\Gamma) = \mu_{k^+}$.

An explicit expression for $\overline{\Gamma}_0(F_1)$ is rather complicated. Namely, $\overline{\Gamma}_0(F_1)$ is the solution of the equation

$$\int_0^1 \frac{\{V(U) - ZF_1(Z-\Gamma) + (3/2)[F_1(Z-\Gamma) - F_1(-\Gamma)]\}\, dU}{Z} = \Gamma$$

where $Z(U) = Z \geqslant 0$ is found from the equation

$$Z^2 + 2ZF_1'(Z - \Gamma) - 2F_1(Z - \Gamma) + 2F_1(-\Gamma) = V(U)$$

3. AN ANALYSIS OF THE PHASE DIAGRAM FOR $\alpha > 0$

We return to the mapping T_0 [see (9)] for positive but small α. Our aim is to find $\gamma_0 = \gamma_0(\alpha) > 1$ such that $1 < \gamma_0(\alpha)$, $\gamma_0(\alpha) - 1 \sim \overline{\Gamma}_0\sqrt{\alpha}$ and $I(\alpha, \gamma) = \mu^{(0)}$ for $1 \leqslant \gamma < \gamma_0(\alpha)$, while $I(\alpha, \gamma) \neq \mu^{(0)}$ for $\gamma > \gamma_0(\alpha)$. The construction of $\gamma_0(\alpha)$ is based on the notion of the homoclinic point.

The point $(0,0) = O$ is a fixed point of the transformation T_0. Under the conditions of Theorem 3 it is a hyperbolic fixed point and thus has stable and unstable separatrices. Let us denote by $\gamma_+^{(s)}, \gamma_+^{(u)} (\gamma_-^{(s)}, \gamma_-^{(u)})$ parts of these separatrices one of whose end points is O, while another end points belong to the half-line $U = \frac{1}{2}$, $Z > 0$ $(Z < 0)$ (see Fig. 3, points $G_+^{(s)}, G_+^{(u)}$, $G_-^{(s)} G_-^{(u)}$).

We construct $T_0^{-1}\gamma_+^{(s)}, T_0^{-1}\gamma_-^{(s)}$ and intersections $T_0^{-1}\gamma_+^{(s)} \cap \gamma_+^{(u)}$. Generically this intersection consists of a finite number of points. The trajectory of each of these points tends to zero as $n \to \pm\infty$. The points with this

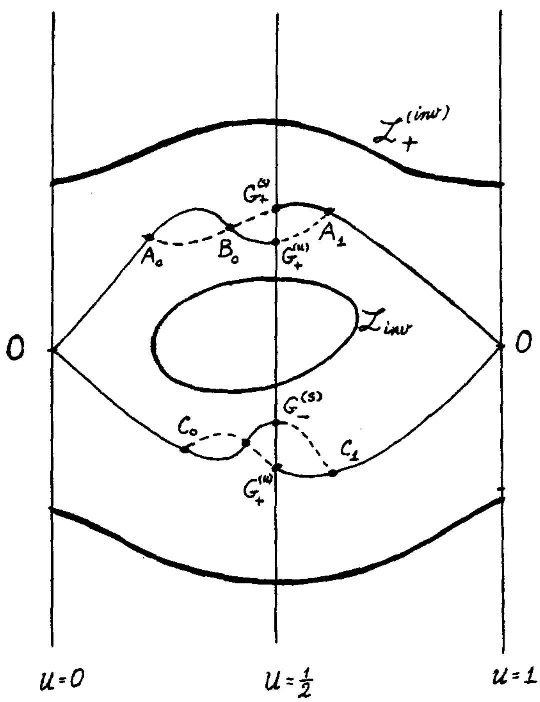


Fig. 3.

property are called homoclinic points (see, e.g., Ref. 11). Assume that $A_0 \in T_0^{-1}\gamma_+^{(s)} \cap \gamma_+^{(u)}$ and $A_k = T_0^k A_0$, $-\infty < k < \infty$. Let us introduce $\gamma_+^{(s)}(0) \subset T_0^{-1}\gamma_+^{(s)}(\gamma_+^{(u)}(0) \subset T_0\gamma_+^{(u)})$ whose end points are A_0 and A_1. If $\gamma_+^{(s)}(0) \cap \gamma_-^{(u)}(0) \neq \emptyset$ then it consists of an odd number of points. Suppose for the sake of simplicity that $\gamma_+^{(s)}(0) \cap \gamma_-^{(u)}(0)$ consists of three points A_0, B_0, A_1. We shall investigate the properties of $\gamma_+^{(s)}(0)$, $\gamma_-^{(u)}(0)$ in more detail. The analysis depends on the assumption that

$$S = \int_{-\infty}^{\infty} \left\{ \frac{V''(U)Z^2}{2} - V'(U)R - R^2\left[1 + ZF_1'''\left(Z - \bar{\Gamma}_0\right) - F_1''\left(Z - \bar{\Gamma}_0\right)\right] \right\} dt \neq 0 \qquad (12)$$

Here $R(U,Z) = V'(U)\{2[1 + F_1''(Z - \Gamma)]\}^{-1}$, $U(t) = U$, $Z(t) = Z > 0$ is the solution of (10) for $\Gamma = \bar{\Gamma}_0(F_1)$ tending to zero as $t \to \pm\infty$. The integral in (12) is an analogy of the well-known Melnikov–Arnold integral in our case (see Refs. 12 and 13). We remark that $S = 0$ if $F_1 = 0$. This fact is the reason why we added F_1 in the expression for F. It is easy to show that the distance between the points $G_+^{(u)}$ and $G_+^{(s)}$ is equal to $S\sqrt{\alpha} + O(\alpha)$ as $\alpha \to 0$. Also homoclinic points are the points of intersection of the stable and unstable separatrices of the point O. It is easy to show that if $S \neq 0$ then the angle between $\gamma^{(s)}$ and $\gamma^{(u)}$ at the points A_0, B_0, A_1 is const $\sqrt{\alpha} + O(\alpha)$, where const $\neq 0$. Now we can formulate explicitly the criterion that $I(\alpha, \gamma) = \mu^{(0)}$, which is the main result of this paper. It was proposed earlier in Refs. 3 and 6 based on the physical considerations. For the points A_0, B_0 we write the following equations for $\bar{\gamma}, \bar{\bar{\gamma}} > 1$:

$$\sum_{-\infty}^{\infty}\left[\frac{1}{2}V\left(\bar{U}_i\right) + \frac{1}{2}\bar{Z}_i^2\right]\sqrt{\alpha} - \frac{\bar{\gamma} - 1}{\sqrt{\alpha}} + \sum_{-\infty}^{\infty}\left[F_1\left(\bar{Z}_i - \frac{\bar{\gamma} - 1}{\sqrt{\alpha}}\right) - F_1\left(-\frac{\bar{\gamma} - 1}{\sqrt{\alpha}}\right)\right]\sqrt{\alpha} = 0 \qquad (13')$$

$$\sum_{-\infty}^{\infty}\left[\frac{1}{2}V\left(\bar{\bar{U}}_i\right) + \frac{1}{2}\bar{\bar{Z}}_i^2\right]\sqrt{\alpha} - \frac{\bar{\bar{\gamma}} - 1}{\sqrt{\alpha}} + \sum_{-\infty}^{\infty}\left[F_1\left(\bar{\bar{Z}}_i - \frac{\bar{\bar{\gamma}} - 1}{\sqrt{\alpha}}\right) - F_1\left(-\frac{\bar{\bar{\gamma}} - 1}{\sqrt{\alpha}}\right)\right]\sqrt{\alpha} = 0 \qquad (13'')$$

Here $(\bar{U}_i, \bar{Z}_i), (\bar{\bar{U}}_i, \bar{\bar{Z}}_i)$ are the coordinates of the points $T_0^i A_0, T_0^i B_0$, $-\infty < i < \infty$.

Lemma 3. $(\bar{\gamma} - 1) \sim \bar{\Gamma}_0(F_1)\sqrt{\alpha}$, $(\bar{\bar{\gamma}} - 1) \sim \bar{\Gamma}_0(F_1)\sqrt{\alpha}$ as $\alpha \to 0$.

The statement of the lemma follows easily from the fact that $\gamma_+^{(u)}, \gamma_+^{(s)}$ tend to the separatrices of the system (10), while the sums in (13′), (13″) tend to the corresponding integrals. We put $\gamma_0(\alpha) = \min(\bar{\gamma}, \bar{\gamma})$ and suppose that all assumptions formulated above are valid.

Theorem 4. For small enough α,

(1) $I(\alpha,\gamma) = \mu^{(0)}$ if $1 \leqslant \gamma < \gamma_0(\alpha)$,

(2) $I(\alpha,\gamma) \neq \mu^{(0)}$ if $\gamma > \gamma_0(\alpha)$.

Proof. Firstly we shall prove (1). Assume that $\gamma < \gamma_0(\alpha)$ and $\mu \neq \mu^{(0)}$ is an ergodic invariant measure for T_0. We shall show that for μ–almost every point (U_0, Z_0) the following inequality is valid:

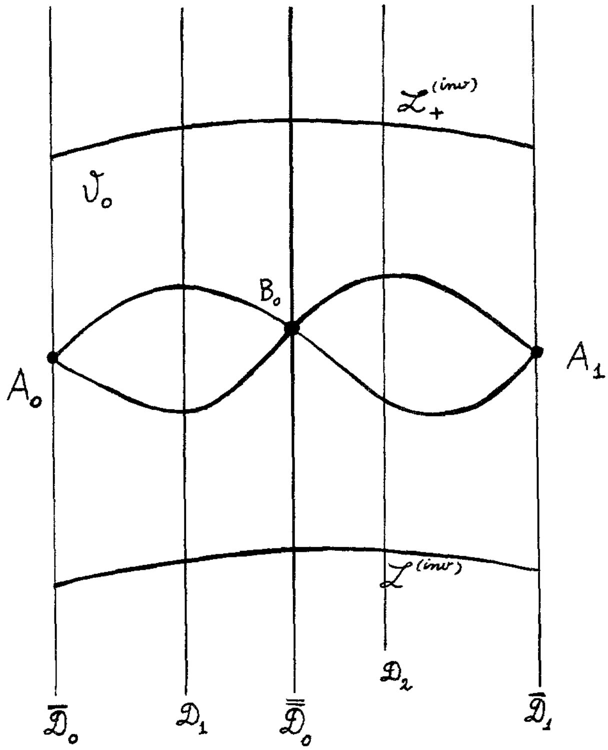
$$\lim_{n\to\infty} \frac{1}{n} \sum_{i=0}^{n} \left[\frac{1}{2} V(U_i) + \frac{1}{2} Z_i^2 + F_1(Z_1 - \Gamma) - F_1(-\Gamma) \right] \sqrt{\alpha} > 0 \quad (14)$$

It is equivalent to the statement of the theorem because it means that

$$\begin{aligned}
&\int \sqrt{\alpha} \left[\frac{1}{2} V(U) + \frac{1}{2} Z^2 - \Gamma Z + F_1(Z - \Gamma) - F_1(-\Gamma) \right] d\mu \\
&= \frac{1}{\sqrt{\alpha}} \left\{ \int \alpha \left[\frac{1}{2} V(U) + \frac{1}{2} (Z - \Gamma)^2 + F_1(Z - \Gamma) \right] d\mu \right. \\
&\qquad \left. - \frac{\alpha}{2} \Gamma^2 - \alpha F_1(-\Gamma) \right\} \\
&= \frac{1}{\sqrt{\alpha}} \left[h(\mu) - h(\mu^{(0)}) \right] > 0
\end{aligned}$$

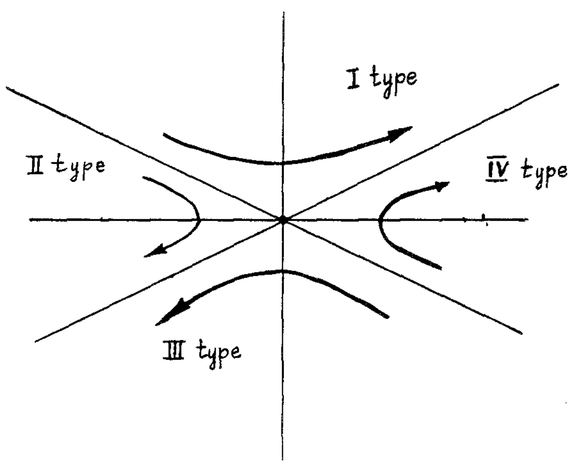
Our proof is based upon the following construction. Let $\overline{\mathfrak{D}}_0$ be the vertical segment of the length $2r$ within the centrum at $(\overline{U}_0, \overline{Z}_0) = A_0$. For $i > 0$ we define the curves $\overline{\mathfrak{D}}_i$, $T_0^i A_0$ is the centrum of $\overline{\mathfrak{D}}_i$, the length of $\overline{\mathfrak{D}}_i$ is equal $2r$, and $T_0 \overline{\mathfrak{D}}_i \supset \overline{\mathfrak{D}}_{i+1}$. In the same way we construct $\overline{\mathfrak{D}}_i$ for $i < 0$, for which $T_0^i A_0 \subset \overline{\mathfrak{D}}_i \subset T_0^{-1} \overline{\mathfrak{D}}_{i+1}$ and similar curves $\overline{\mathfrak{D}}_i$ passing through the points $T_0^i B_0$, $-\infty < i < \infty$. Also we construct two vertical segments $\mathfrak{D}_1, \mathfrak{D}_2$ between $\overline{\mathfrak{D}}_0, \overline{\mathfrak{D}}_0$ and $\overline{\mathfrak{D}}_0, \overline{\mathfrak{D}}_1$, respectively, in such a way that the distances between $\mathfrak{D}_1, \mathfrak{D}_2$ and $\overline{\mathfrak{D}}_0, \overline{\mathfrak{D}}_0, \overline{\mathfrak{D}}_1$ were of the same order (see Fig. 4). KAM theory is applied to our case and it gives the existence of invariant curves $\mathfrak{L}_+^{(\mathrm{inv})}$ above $\gamma_+^{(u)}, \gamma_+^{(s)}$, $\mathfrak{L}_-^{(\mathrm{inv})}$ below $\gamma_-^{(u)}, \gamma_-^{(s)}$ and $\mathfrak{L}^{(\mathrm{inv})}$ between them (see Fig. 3). In particular these curves can be chosen arbitrarily close to the separatrices of the system (10) provided α is sufficiently small. We denote ϑ_0 the domain bounded by $\overline{\mathfrak{D}}_0, \overline{\mathfrak{D}}_1$ and the parts of the curves $\mathfrak{L}_+^{(\mathrm{inv})}, \mathfrak{L}^{(\mathrm{inv})}$.

We consider the most difficult case when the measure μ is concentrated in the domain bounded by $\mathfrak{L}_+^{(\mathrm{inv})}$, $\mathfrak{L}_-^{(\mathrm{inv})}$, and $\mathfrak{L}^{(\mathrm{inv})}$. Let us fix a neighborhood Q of the fixed pont O not depending on α. Each trajectory of T_0 which is not a homoclinic one enters Q infinitely many times and then



$\mathcal{L}_+^{(inv)}$
ϑ_0
B_0
A_0
A_1
$\mathcal{L}^{(inv)}$
$\mathcal{D}_2$
$\bar{\mathcal{D}}_0$
$\mathcal{D}_1$
$\bar{\bar{\mathcal{D}}}_0$
$\bar{\mathcal{D}}_1$

Fig. 4.



I type
II type
IV type
III type

Fig. 5.

goes out of it. During each visit of Q it intersects one of four coordinate segments in Q having O as an origin. Let us denote $0 < i_1 < i_2 < \cdots < i_s < \cdots$ the successive moments of these intersections. It is obvious that each i_s can be of one of the following types (see Fig. 5):

I type: $Z_{i_s} > 0, \quad U_{i_s} < 0, \quad U_{i_{s+1}} > 0$

II type: $U_{i_s} < 0, \quad Z_{i_s} > 0, \quad Z_{i_{s+1}} \leqslant 0$

III type: $Z_{i_s} < 0, \quad U_{i_s} > 0, \quad U_{i_{s+1}} \leqslant 0$

IV type: $U_{i_s} > 0, \quad Z_{i_s} < 0, \quad Z_{i_{s+1}} \geqslant 0$

The segment $i_s < i \leqslant i_{s+1}$ is the segment of kth type if i_s has the kth type, $k = \mathrm{I, II, III, IV}$. We shall denote the type of the sth segment as k_s. A segment of the IVth type can follow after segments of the II and III types, a segment of the type I can follow after segments of the types I and IV, a segment of the type II can follow after segments of the types I and IV, and a segment of the third type can follow after segments of the types III and II. Also from the equality $U_{i+1} - U_i = \sqrt{\alpha}\, Z_{i+1}$ we get

$$\sum_{i=i_{s-1}+1}^{i_s} Z_i = \frac{\kappa_s}{\sqrt{\alpha}} + \frac{U_{i_s} - U_{i_{s-1}}}{\sqrt{\alpha}}$$

where $\kappa_s = 1$ in the case of the I and IV types and -1 in the other cases. It shows that in the sum (14)

$$\lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^{n} Z_i = \lim_{s\to\infty} \frac{1}{i_s} \sqrt{\alpha} \sum_{p=0}^{s-1} \kappa_p \tag{15}$$

Now we put $W(U,Z) = \{\frac{1}{2} V(U) + \frac{1}{2} Z^2 + [F_1(Z-\Gamma) - F_1(-\Gamma)]\}$ and write

$$\begin{aligned}
\sum_s = \sum_{i=0}^{i_s} \left[W(U_i, Z_i) - \Gamma Z_i \right] &= \sum_{i=0}^{i_s} \left[W(U_i, Z_i) - \Gamma Z_i \right] \\
&+ \sum_{t\,:\,k_t = \mathrm{I}, k_{t+1} = \mathrm{I}} \sum_{i=i_t+1}^{i_{t+1}} W(U_i, Z_i) + \sum_{t\,:\,k_t = \mathrm{I}, k_{t+1} = \mathrm{II}} \sum_{i=i_t+1}^{i_{t+2}} W(U_i, Z_i) \\
&+ \sum_{t\,:\,k_{t-1} = \mathrm{II}, k_t = \mathrm{IV}, k_{t+1} = \mathrm{II}} \sum_{i=i_t+1}^{i_{t+2}} W(U_i, Z_i) \\
&+ \sum_{t\,:\,k_{t-1} = \mathrm{III}, k_t = \mathrm{IV}, k_{t+1} = \mathrm{I}} \left[\sum_{i=i_t+1} W(U_i, Z_i) - \Gamma \right] \\
&+ \sum_{t\,:\,k_{t-1} = \mathrm{II}, k_t = \mathrm{III}} \left[\sum_{i=i_t+1}^{i_{t+1}} W(U_i, Z_i) + \Gamma \right] \\
&+ \sum_{t\,:\,k_{t-1} = \mathrm{III}, k_t = \mathrm{III}} \left[\sum_{i=i_t+1}^{i_{t+1}} W(U_i, Z_i) + \Gamma \right]
\end{aligned}$$

Under our conditions on F_1 the inner sums in the third, fourth, sixth, and seventh sums are strictly positive, i.e., are more than a const. The first sum does not depend on s and can be neglected. Concerning the fifth sum our analysis will show that it can be done arbitrarily small provided α, Q, and ϑ are sufficiently small while the previous sum $\sum_{i=i_{t-1}+1}^{i_t} W(U_i, Z_i) + \Gamma$ is always more then a const. Thus the sum of all terms except the second one is positive and we have to consider only the expressions

$$\sum_{i=i_t+1}^{i_{t+1}} {}^{(1)}\left[W(U_i, Z_i) \right] - \Gamma$$

for the case $k_t = I$, $k_{t+1} = I$.

It is convenient to change the summation index and to suppose that i changes between $i^- < 0$ and $i^+ > 0$, $i^+ - i^- = i_{t+1} - i_t$ and for $i = 0$ the point $(U_0, Z_0) \in \vartheta_0$. Also we assume that (U_0, Z_0) lies between $\overline{\mathfrak{D}}_0$ and $\mathfrak{D}_1$. If (U_0, Z_0) lies between $\mathfrak{D}_1$ and $\mathfrak{D}_2$ ($\mathfrak{D}_2$ and $\overline{\mathfrak{D}}_1$) we shall compare its trajectory with the trajectory of B_0 (A_1); see below. Under the conditions of the theorem

$$\sum_{i=-\infty}^{\infty} W(\overline{U}_i, \overline{Z}_i) - \Gamma > 0$$

We shall show that

$$\Sigma^{(1)} = \sum_{i=i^-}^{i^+} \left[W(U_i, Z_i) - W(\overline{U}_i, \overline{Z}_i) \right]$$

$$- \sum_{i>i^+} W(\overline{U}_i, \overline{Z}_i) - \sum_{i<i^-} W(\overline{U}_i, \overline{Z}_i) > 0 \tag{16}$$

which obviously leads to the statement of the theorem. We shall use the notation $Y = Z + F_1'(Z - \Gamma)$ and the equalities which follow partly from the definition of T_0 [see (9)]:

$$V(U_i) - V(\overline{U}_i) = V'(\overline{U}_i)(U_i - \overline{U}_i) + \tfrac{1}{2} V''(\overline{U}_i)(U_i - \overline{U}_i)^2$$

$$+ R_i^{(1)}(U_i - \overline{U}_i)^3$$

$$V'(U_i) - V'(\overline{U}_i) = V''(\overline{U}_i)(U_i - \overline{U}_i) + R_i^{(2)}(U_i - \overline{U}_i)^2 \tag{17}$$

$$V''(\overline{U}_i)(U_i - \overline{U}_i)^2 = \left[V'(U_i) - V'(\overline{U}_i) \right](U_i - \overline{U}_i) - R_i^{(2)}(U_i - \overline{U}_i)^3$$

$$V'(\overline{U}_i) = \frac{2}{\sqrt{\alpha}} (\overline{Y}_{i+1} - \overline{Y}_i), \qquad V'(U_i) = \frac{2}{\sqrt{\alpha}} (Y_{i+1} - Y_i)$$

Here $|R_i^{(1)}|, |R_i^{(2)}| \leqslant$ const. Now we can write

$$\begin{aligned}
\Sigma^{(2)} &= \sum_{i=i^-}^{i^+} \left[W(U_i, Z_i) - W(\bar{U}_i, \bar{Z}_i) \right] \\
&= \sum_{i=i^-}^{i^+} \Big\{ \tfrac{1}{2}\left[V(U_i) - V(\bar{U}_i) \right] + (Z_i - \bar{Z}_i)\bar{Z}_i \\
&\qquad + \tfrac{1}{2}(Z_i - \bar{Z}_i)^2 + F_1(Z_i - \Gamma) - F_1(\bar{Z}_i - \Gamma) \Big\} \\
&= \sum_{i=i^-}^{i^+} \Big[\tfrac{1}{2} V'(\bar{U}_i)(U_i - \bar{U}_i) + \tfrac{1}{4} V''(\bar{U}_i)(U_i - \bar{U}_i)^2 + (Z_i - \bar{Z}_i)\bar{Z}_i \\
&\qquad + \tfrac{1}{2}(Z_i - \bar{Z}_i)^2 F_1(Z_i - \Gamma) + F_1(\bar{Z}_i - \Gamma) \Big] + \Sigma^{(3)} \\
&= \sum_{i=i^-}^{i^+} \Big[(1/\sqrt{\alpha})(\bar{Y}_{i+1} - \bar{Y}_i)(U_i - \bar{U}_i) + \tfrac{1}{4}\left[V'(U_i) - V'(\bar{U}_i) \right](U_i - \bar{U}_i) \\
&\qquad + (Z_i - \bar{Z}_i)\bar{Z}_i + \tfrac{1}{2}(Z_i - \bar{Z}_i)^2 + F_1(Z_i - \Gamma) - F_1(\bar{Z}_i - \Gamma) \Big] \\
&\quad + \Sigma^{(3)} - \Sigma^{(4)} = \Sigma_1^{(2)} + \Sigma^{(3)} - \Sigma^{(4)}
\end{aligned}$$

Here $\Sigma^{(3)} = \Sigma R_i^{(1)}(U_i - \bar{U}_i)^3$, $\Sigma^{(4)} = \frac{1}{4}\Sigma R_i^{(2)}(U_i - \bar{U}_i)^3$ and will be treated as remainder terms. We continue now the analysis of $\Sigma_1^{(2)}$:

$$\begin{aligned}
\Sigma_1^{(2)} &= \sum_{i=i^-}^{i^+} \Big\{ \frac{1}{\sqrt{\alpha}}(\bar{Y}_{i+1} - \bar{Y}_i)(U_i - \bar{U}_i) + \tfrac{1}{4}\left[V'(U_i) - V'(\bar{U}_i) \right](U_i - \bar{U}_i) \\
&\qquad + (Z_i - \bar{Z}_i)\bar{Z}_i + \tfrac{1}{2}(Z_i - \bar{Z}_i)^2 + F_1(Z_i - \Gamma) - F_1(\bar{Z}_i - \Gamma) \Big\} \\
&= \sum_{i=i^-}^{i^+} \Big[\frac{1}{\sqrt{\alpha}} \bar{Y}_i (U_{i-1} - \bar{U}_{i-1} - U_i + \bar{U}_i) \\
&\qquad + \frac{1}{2\sqrt{\alpha}}(Y_{i+1} - Y_i - \bar{Y}_{i+1} + \bar{Y}_i) \\
&\qquad \times (U_i - \bar{U}_i) + (Z_i - \bar{Z}_i)\bar{Z}_i + \tfrac{1}{2}(Z_i - \bar{Z}_i)^2 \\
&\qquad + F_1(Z_i - \Gamma) - F_1(\bar{Z}_i - \Gamma) \Big] \\
&\quad + \frac{1}{\sqrt{\alpha}} \bar{Y}_{i^+ + 1}(U_{i^+ + 1} - \bar{U}_{i^+ + 1}) - \frac{1}{\sqrt{\alpha}} \bar{Y}_{i^-}(U_{i^- - 1} - \bar{U}_{i^- - 1})
\end{aligned}$$

The first sum is denoted by $\Sigma_2^{(2)}$. We have

$$\Sigma_2^{(2)} = \sum_{i=i^-}^{i^+} \Big[\overline{Y}_i(\overline{Z}_i - Z_i) + \frac{1}{2\sqrt{\alpha}}(\overline{Y}_i - Y_i)(U_i - \overline{U}_i - U_{i-1} + \overline{U}_{i-1})$$

$$+ (Z_i - \overline{Z}_i)\overline{Z}_i + \tfrac{1}{2}(Z_i - \overline{Z}_i)^2 + F_1(Z_i - \Gamma) - F_1(\overline{Z}_i - \Gamma)\Big]$$

$$- \frac{1}{2\sqrt{\alpha}}(\overline{Y}_{i^+ + 1} - Y_{i^+ + 1})(U_{i^+} - \overline{U}_{i^+})$$

$$+ \frac{1}{2\sqrt{\alpha}}(\overline{Y}_{i^-} - Y_{i^-})(U_{i^- - 1} - \overline{U}_{i^- - 1})$$

The sum in the last expression is denoted by $\Sigma_3^{(3)}$. The final step is the following:

$$\Sigma_3^{(2)} = \sum_{i=i^-}^{i^+} \Big[F_1(Z_i - \Gamma) - F_1(\overline{Z}_i - \Gamma) - F_1'(\overline{Z}_i - \Gamma)(Z_i - \overline{Z}_i)$$

$$+ \tfrac{1}{2}(\overline{Y}_i - Y_i)(Z_i - \overline{Z}_i) + \tfrac{1}{2}(Z_i - \overline{Z}_i)^2\Big]$$

$$= \sum_{i=i^-}^{i^+} \Big\{ F_1(Z_i - \Gamma) - F_1(\overline{Z}_i - \Gamma) - F_1'(\overline{Z}_i - \Gamma)(Z_i - \overline{Z}_i)$$

$$- \tfrac{1}{2}\big[F_1'(Z_i - \Gamma) - F_1'(\overline{Z}_i - \Gamma)\big](Z_i - \overline{Z}_i)\Big\}$$

$$= \sum_{i=i^-}^{i^+} R_i^{(3)}(Z_i - \overline{Z}_i)^3$$

Here $|R_i^{(3)}| \leqslant \max_Z |F_1'''(Z)| \leqslant \text{const}$ and the last expression is also a remainder term. Finally we get

$$\Sigma^{(1)} = \frac{1}{\sqrt{\alpha}} \overline{Y}_{i^+ + 1}(U_{i^+ + 1} - \overline{U}_{i^+ + 1}) + \frac{1}{2\sqrt{\alpha}}(Y_{i^+ + 1} - \overline{Y}_{i^+ + 1})(U_{i^+} - \overline{U}_{i^+})$$

$$- \frac{1}{\sqrt{\alpha}} \overline{Y}_{i^-}(\overline{U}_{i^- - 1} - U_{i^- - 1}) + \frac{1}{2\sqrt{\alpha}}(Y_{i^-} - \overline{Y}_{i^-})(\overline{U}_{i^- - 1} - U_{i^- - 1})$$

$$+ \Sigma^{(3)} - \Sigma^{(4)} + \Sigma_3^{(2)} - \sum_{i > i^+} W(\overline{U}_i, \overline{Z}_i) - \sum_{i < i^-} W(\overline{U}_i, \overline{Z}_i)$$

We shall show that the first four terms are in a sense larger than the others. It is easy to see that $|\Sigma^{(3)}|, |\Sigma^{(4)}| \leqslant \text{const}\, \alpha^{-1/2}|U_0 - \overline{U}_0|^3$, $\Sigma_3^{(2)} \geqslant -\text{const}\, \alpha^{-1/2}|U_0 - \overline{U}_0|^3$. We shall use the estimations which follow easily from the fact that $O = (0,0)$ is a hyperbolic fixed point of T_0:

$$\left.\frac{d\gamma^{(s)}}{dU}\right|_{U=0} = -R\big[1 + O(\sqrt{\alpha})\big], \qquad \left.\frac{d\gamma^{(u)}}{dU}\right|_{U=0} = R\big[1 + O(\sqrt{\alpha})\big]$$

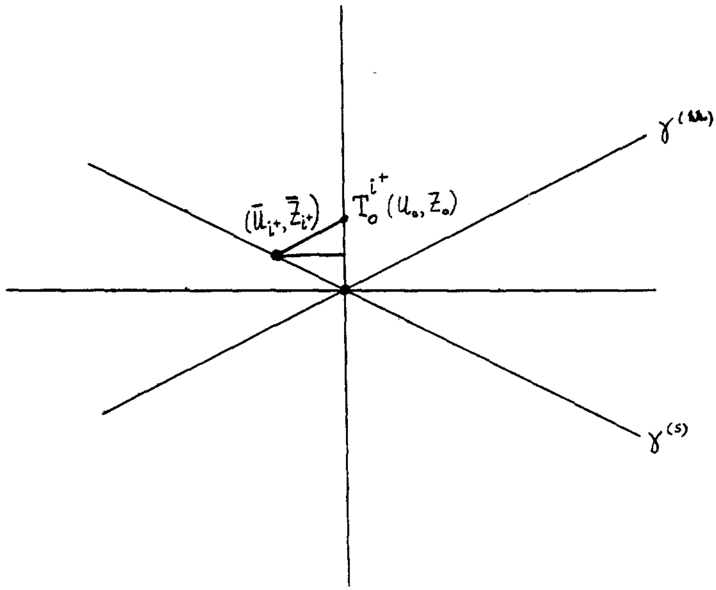


Fig. 6.

where $R = (V''(0)\{2[1 + F_1''(-\Gamma)]\})^{-1}$. The transformation T_0 is a hyperbolic rotation with the expansion coefficient $(1 + R\sqrt{\alpha} + O(\alpha))$ along $\gamma^{(u)}$ and with the contraction coefficient $(1 - R\sqrt{\alpha} + O(\alpha))$ along $\gamma^{(s)}$.

This leads to the following conclusions (see Fig. 6):

$$Z_{i^+1} - \overline{Z}_{i^++1} \sim \tfrac{1}{2}\overline{Z}_{i^+}, \qquad Z_i^- - \overline{Z}_{i^-} \sim \tfrac{1}{2}\overline{Z}_{i^-}$$

$$U_{k^++1} - \overline{U}_{i^++1} \sim -\overline{U}_{i^+} \sim R^{-1}\overline{Z}_{i^+}$$

$$U_{i^--1} - \overline{U}_{i^--1} \sim \overline{U}_{i^-} \sim R^{-1}\overline{Z}_{i^-}$$

Also we denote $\max_{|Z|\leqslant 2\Gamma_1}|F_1'(Z)| = \mathcal{F}_1'$, $\max_{|Z|\leqslant 2\Gamma_1} F_1''(Z) = \mathcal{F}_1''$. Using all relations we can write

$$\frac{1}{\sqrt{\alpha}}\,\overline{Y}_{i^++1}\big(U_{i^++1} - \overline{U}_{i^++1}\big) + \frac{1}{2\sqrt{\alpha}}\big(Y_{i^++1} - \overline{Y}_{i^++1}\big)\big(U_{i^+} - \overline{U}_{i^+}\big)$$

$$\sim \frac{\overline{Z}_{i^+}^2}{\sqrt{\alpha}\,R} + \frac{\overline{Z}_{i^+}^2}{4\sqrt{\alpha}\,R} + \frac{1}{\sqrt{\alpha}\,R}F_1'(-\Gamma)\overline{Z}_{i^+} + \frac{1}{2\sqrt{\alpha}\,R}F_1'(-\Gamma)\overline{Z}_{i^+}^2$$

$$= \frac{5}{4\sqrt{\alpha}\,R}\overline{Z}_{i^+}^2 + \frac{1}{\sqrt{\alpha}\,R}F_1'(-\Gamma)\cdot\overline{Z}_{i^+} + \frac{1}{2\sqrt{\alpha}\,R}F_1'(-\Gamma)\overline{Z}_{i^+}^2 \qquad (18)$$

From the other side

$$\sum_{i>i^+}\left[\tfrac{1}{2}V(\bar{U}_i)+\tfrac{1}{2}\bar{Z}_i^2+F_1(\bar{Z}_i-\Gamma)-F_1(-\Gamma)\right]$$

$$=\sum_{i>i^+}\left[\tfrac{1}{4}V''(0)\bar{U}_i^2+\tfrac{1}{2}\bar{Z}_i^2+F_1'(-\Gamma)\bar{Z}_i+\tfrac{1}{2}F_1''(\theta_i)\bar{Z}_i^2+\cdots\right]$$

The last sum can be estimated easily from above by the expression

$$\frac{V''(0)}{4R\sqrt{\alpha}}\bar{U}_{i^+}^2+\frac{1}{2R\sqrt{\alpha}}\bar{Z}_{i^+}^2+F_1'(-\Gamma)\bar{Z}_{i^+}\cdot\frac{1}{R\sqrt{\alpha}}+\frac{\text{const}}{R\sqrt{\alpha}}(\mathcal{F}_1'+\mathcal{F}_1'')\bar{Z}_{i^+}^2 \quad (19)$$

Here const in the last term tends to a finite limit as $\mathcal{F}_1',\mathcal{F}_1''\to 0$. Thus it can be considered as an absolute constant. Now we replace (19) by an equivalent expression

$$\left[\frac{V''(0)}{4R^3\sqrt{\alpha}}+\frac{1}{2R\sqrt{\alpha}}\right]=\bar{Z}_{i^+}^2+F_1'(-\Gamma)\frac{\bar{Z}_{i^+}}{R\sqrt{\alpha}}+\frac{\text{const}(\mathcal{F}_1'+\mathcal{F}_2'')}{R\sqrt{\alpha}}\cdot\bar{Z}_{i^+}^2$$

We remark that

$$\frac{V''(0)}{4R^3\sqrt{\alpha}}+\frac{1}{2R\sqrt{\alpha}}=\frac{1}{2R\sqrt{\alpha}}\left[\frac{V''(0)}{2R^2}+1\right]=\frac{1}{R\sqrt{\alpha}}\left[1+\frac{1}{2}F_1''(-\Gamma)\right] \quad (20)$$

If $\mathcal{F}_1',\mathcal{F}_1''$ are sufficiently small than for sufficiently small α the difference between (18) and (20) is not less than

$$\frac{1}{4R\sqrt{\alpha}}\cdot(1-\mathcal{F})\bar{Z}_{i^+}^2$$

where $\mathcal{F}\to 0$ as $\mathcal{F}_1',\mathcal{F}_1''\to 0$.

In the same manner we can treat the terms containing $U_i,\bar{U}_i,Z_i,\bar{Z}_i$ for $i<i^-$. As a result we get

$$\Sigma^{(1)}\geqslant\frac{1}{4\sqrt{\alpha}\,R}(1-\mathcal{F})\bar{Z}_{i^+}^2+\frac{1}{4\sqrt{\alpha}\,R}(1-\mathcal{F})\bar{Z}_{i^-}^2-\frac{\text{const}}{\sqrt{\alpha}}|U_0-\bar{U}_0|^3 \quad (21)$$

The value of $Z_{i^+}(Z_{i^-})$ depends on the distance between (U_0,Z_0) and $\gamma^{(s)}(\gamma^{(u)})$ (see Fig. 4). Assume that $Z=\Phi^{(s)}(U), Z=\Phi^{(u)}(U)$ are functions which define $\gamma^{(s)},\gamma^{(u)}$ in ϑ. We put $\Delta^{(s)}=Z_0-\Phi^{(s)}(U_0)$, $\Delta^{(u)}=Z_0-\Phi^{(u)}(U_0)$. For the segments of the type I we have $\Delta^{(s)}>0,\Delta^{(u)}>0$. It is easy to show that $Z_{i^+}^2\sim\text{const}\,\Delta^{(s)}$, $Z_{i^-}^2\sim\text{const}\,\Delta^{(u)}$. The angle between $\gamma^{(s)},\gamma^{(u)}$ at their points of intersection is not less than const $\sqrt{\alpha}$ (see above).

Therefore $\max(\Delta^{(s)}, \Delta^{(u)}) \geqslant \text{const}\sqrt{\alpha}\,|U_0 - \overline{U}_0|$. Finally we get [see (21)]

$$\begin{aligned}\Sigma^{(1)} &\geqslant \frac{\text{const}}{4\sqrt{\alpha}\,R}\max(\Delta^{(s)}, \Delta^{(u)}) - \frac{\text{const}}{\sqrt{\alpha}}\,|U_0 - \overline{U}_0|^3 \\ &\geqslant \frac{\text{const}}{4R}\,|U_0 - \overline{U}_0| - \frac{\text{const}}{\sqrt{\alpha}}\,|U_0 - \overline{U}_0|^3 \\ &= |U_0 - \overline{U}_0|\left(\frac{\text{const}}{4R} - \frac{\text{const}}{\sqrt{\alpha}}\,|U_0 - \overline{U}_0|^2\right)\end{aligned}$$

Now we remark that $|U_0 - \overline{U}_0| \leqslant \text{const}\sqrt{\alpha}$ because the distance between A_0 and A_1 is of order $\sqrt{\alpha}$. Therefore the last expression is not less than

$$|U_0 - \overline{U}_0|\left(\frac{\text{const}}{4R} - \text{const}\sqrt{\alpha}\right) > 0$$

for sufficiently small α.

For other measures μ the statement of the theorem follow easily from its validity for $\alpha = 0$.

Now we pass to the second statement of the theorem. According to the Poincaré–Smale–Shilnikov theorem (see Ref. 11) in small neighborhoods of A_0, B_0 there exist periodic points which make one turn around the cylinder C, i.e., $\sum(U_{i^+ + 1} - U_{i^+}) = 1$. For such trajectories the sum

$$\sum\left[V(U_i) + Z_i^2 + F_1(Z_i - \Gamma) - F_1(-\Gamma)\right] - 2\Gamma$$

tends to the similar sum for the homoclinic point and therefore will be eventually negative in view of conditions of the theorem. Let μ be a normed measure concentrated on this periodic trajectory. Then $h(\mu) - h(\mu^{(0)}) < 0$. ∎

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