Chirikov criterion of resonance overlapping for the model of molecular dynamics

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The chaotic dynamics in a cell of particles’ chain interacting by means of Lennard-Jones potential is considered. Chirikov criterion of resonance overlapping is used as the condition of chaos. The asymptotic representation for this function at low and high energies is obtained for the function corresponding to the criterion.

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Introduction

It is well known [1] that investigation of the problem occurrence of chaotic dynamics naturally led to the need to study simple models in which there is chaos. Further study of the real physical processes in which there is chaos showed that many simple models reflect its main, for example, the occurrence of stochastic separatrix layer, formation of nonlinear resonances and etc.

One-dimensional chains of particles have also been the subject of research in studying the problems of chaotic dynamics [1] because some problems for them are reduced to the study of standard maps known for nonlinear dynamic systems. On the other hand investigation of the phenomena of chaos chain of particles is also important in connection with the active use of the particle method for simulating the behavior of materials. Speaking about this method we consider the particles as point masses, and not as discrete elements allowing to reduce the equations of continuum mechanics to the difference system of ordinary differential equations. One of the most well-developed variants of the particle method is the method of molecular dynamics in the classical version of which particles act as atoms and molecules. If interatomic potential is known then the dynamics of molecular compounds can be modeled with high accuracy.

Despite the good correlation between the results of computer simulation observed experiment and material behavior there is a problem of understanding their internal mechanisms in terms of nonlinear dynamics. For one-dimensional system corresponding model problem is reduced to consideration of the particle mass \( m \) in the cell. The dynamics of particle is determined by
the Hamiltonian

\[ H = H(p, q, t) = \frac{p^2}{2m} + V(q), \quad V(q) = U(q) + U(\xi(t) - q), \quad (1) \]

in which \( p \) is the particle momentum, and form of the function \( \xi(t) \) depends on the collective behavior of particles in the system. Formula (1) means that particle interacts with a stationary particle on the left side and interacts with a particle moving in a law \( q_2 = \xi(t) \) on the right one. The interaction between the particles is characterized by the potential \( U(q) \).

The phenomenon of strong chaos for particles interacting by means of the Lennard-Jones potential \( U(q) \) was considered in [2]. Chirikov criterion of resonance overlapping [3] was used as the condition of chaos. The function \( K_{n,n-1} \) corresponding to the criterion was calculated numerically with respect to energy. In this article we obtain the asymptotic representation for this function at low and high energies.

1 Chirikov criterion of resonance overlapping

Let us remind the model [2]. Interaction is determined by the Lennard-Jones potential \( U(q) = U_0 \left\{ \left( \frac{a}{q} \right)^\alpha - \frac{\alpha}{\beta} \left( \frac{a}{q} \right)^\beta \right\} \) with \( \alpha > \beta > 0 \). The perturbation \( \xi(t) \) is given by the formula \( \xi(t) = 2a(1 + \varepsilon(t)), \quad \varepsilon(t) = \alpha_1 \cos \omega_1 t \) with \( |\alpha_1| \ll 1 \). We introduce the dimensionless variables setting \( H \rightarrow H/U_0, \quad q \rightarrow q/a - 1, \quad t \rightarrow t/t_0, \quad \omega_1 \rightarrow \omega_1 t_0 \) where \( t_0 = \sqrt{ma^2/U_0} \). Then Hamiltonian (1) is written in the form

\[ H(p, q, t) = \frac{p^2}{2} + V(q), \quad V(q) = U(q + 1) + U(1 + \varepsilon(t) - q). \quad (2) \]

Given the small amplitude \( \varepsilon(t) \) we carry out the expansion of the Hamiltonian (2) with respect to \( \varepsilon(t) \):

\[ H(p, q, t) = H_0(p, q) - \varepsilon(t)H_1(q) + \ldots, \]
\[ H_0(p, q) = \frac{p^2}{2} + W(q), \quad H_1(q) = \frac{dU}{dq}(1-q), \quad W(q) = U(q+1) + U(q-1). \quad (3) \]

Action-angle variables \((I, \varphi)\) are commonly used in studying the dynamics of Hamiltonian systems [1]. The unperturbed action is conserved along the phase trajectory and its value is determined by initial conditions \((p_0, q_0)\). If you choose \( p_0 = 0 \) the correspondence between the unperturbed action \( I \) and the parameter \( q_0 \) is unique. Transformation to the action-angle variables can
be carried out numerically in accordance with formulae

\[ I(q_0) = \frac{2}{\pi} \int_0^{q_0} p(q_0, q) dq, \quad \varphi(q, q_0) = \omega \int_{q_0}^{q} \frac{dq}{p(q_0, q)}, \quad \omega = \frac{\pi}{2 \int_0^{q_0} \frac{dq}{p(q_0, q)}}, \quad (4) \]

where \( p(q_0, q) = \sqrt{2(V(q_0) - V(q))} \). We express the variables \((p, q)\) in the terms of \((I, \varphi)\). Then Hamiltonian \( H(p, q, t) \) can be expanded in a Fourier series:

\[ H(p, q, t) = H_0(I) - \frac{1}{2} \alpha_1 \sum_n H_n(I)[\cos(n\varphi + \varphi_0 - \omega_1 t) + \cos(n\varphi + \varphi_0 + \omega_1 t)], \quad (5) \]

Let us consider the resonance condition for a three of numbers \((n, I_n, \omega_1)\):

\[ n\omega(I_n) = \omega_1. \]

To analyze the dynamics of the system in the vicinity of nonlinear resonance we use the standard method [1]. In this case the only resonant harmonic in \((5)\) is fixed:

\[ H(p, q, t) = H_0(I) - \frac{1}{2} \alpha_1 H_n(I) \cos(n\varphi + \varphi_0 - \omega_1 t). \quad (6) \]

We introduce a new phase \( \psi = n\varphi + \varphi_0 - \omega_1 t \) then the equations of motion corresponding to Hamiltonian \((6)\) have the form

\[ \frac{dI}{dt} = -\frac{\partial H}{\partial \psi} = \frac{1}{2} \alpha_1 H_n(I) \sin \psi, \]

\[ \frac{d\psi}{dt} = \frac{\partial H}{\partial I} = n\omega(I) - \omega_1 - \frac{1}{2} \alpha_1 \cos \psi \frac{d}{dt} H_n(I). \quad (7) \]

As the equations \((7)\) are examined in the vicinity of the resonance action \( I_{n1} \) it is assumed that the value \( J = I - I_n \) is small. We expand \( H_0(I), \omega(I) \) and neglect the terms \( J^2 \) correspondingly. Then the equations \((7)\) are written in the form:

\[ \frac{dJ}{dt} = \frac{1}{2} \alpha_1 H_n(I_n) \sin \psi, \quad \frac{d\psi}{dt} = nJ \frac{d\omega}{dI}(I_n). \]

The obtained equations correspond to the so-called nonlinear pendulum Hamiltonian [1]:

\[ H(J, \psi) = n \frac{J^2}{2} \frac{d\omega}{dI}(I_n) - \frac{1}{2} \alpha_1 H_n(I_n) \cos \psi. \]
The width of the resonance $\Delta J$ is calculated from the condition:

$$\frac{(\Delta J)^2}{2} \frac{d\omega}{dI}(I_n) = \frac{1}{2} \alpha_1 H_n(I_n); \quad \Delta J = \sqrt{\frac{\alpha_1 H_n(I_n)}{\frac{d\omega}{dI}(I_n)}}. \tag{1}$$

In terms of frequency $\omega$ we have

$$\Delta \omega \approx \sqrt{\frac{1}{2} \alpha_1 H_n(I_n) \frac{d\omega}{dI}(I_n)}. \tag{8}$$

Consider the invariant curves for the resonant action $I_n, I_{n-1}$. In order to form a chaotic region in the plane $(p,q)$ it is necessary to destroy the curves corresponding to these values of the action. Let us assume that $\Delta \Omega (\Delta I)$ is the corresponding width of the resonance and $\delta \Omega = \omega(I_n) - \omega(I_{(n-1)}) \quad (\delta I = I_n - I_{(n-1)})$ is the distance between resonances. The parameter $K$ characterizing the degree of resonance overlapping is equal to $K = \Delta I/\delta I \approx \Delta \Omega/\delta \Omega$ [1]. In accordance to Chirikov criterion [3] the overlap of resonance takes place on condition that $|K| \geq 1$:

$$K_{n,n-1}(q_0(\omega_1)) = \frac{\Delta \omega(I_n) + \Delta \omega(I_{(n-1)})}{\omega(I_n) - \omega(I_{(n-1)})} \sim 1. \tag{9}$$

In [2] the function $K_{3,2}$ was calculated numerically at different $|\alpha_1| \ll 1$ with respect to $q_0$ (energy). In this article we construct an asymptotic representation for the functions $K_{1,2}(q_0(\omega_1)), K_{2,3}(q_0(\omega_1))$ at small and large energies.

### 2 Approximate action-angle variables at small energy

The criterion (1) includes the frequency and its derivative (3), and the value of the Fourier coefficient (5). From the point of view of physics the smallness of the energy values correspond to the fulfillment of the inequality $E \ll 1$. This allows us to use an approximation for $W(q)$ (3) as polynomial functions with respect to $q$ and construct approximate formulae for the action-angle variables at $E \to 0$. Approximation for the potential $W$ is obtained after expansion in the vicinity of the point $q = 0$:

$$W_{app}(q) = W_0 + bq^2 + cq^4, \quad b = U^{(2)}(1), \quad c = \frac{U^{(4)}(1)}{12}. \tag{10}$$

Let us introduce the approximate action-angle variables assuming

$$J(E) = \frac{1}{\pi} \int_{Q_1}^{Q_2} p_{app} dq, \quad \psi = \Omega t_{app}, \quad t_{app} = \int_{Q_1}^{q} \frac{dq}{p_{app}}$$
where \( p_{\text{app}} = \sqrt{2(E - W_{\text{app}}(q))} \), and the coordinates of points \( Q_i \) are determined from the equation \( E = W_{\text{app}}(Q_i) \). The quantity \( \Omega = \frac{\partial E}{\partial J} = \frac{\pi}{T(E)} \) is the cyclic frequency where \( T(E) \) is the period of motion in the potential \( (10) \). Omitting simple calculations we have the following presentation for \( T(E) \):

\[
\frac{T}{2} = \int_{Q_1}^{Q_2} \frac{dq}{\sqrt{2(E - W_{\text{app}}(q))}} = \frac{1}{\sqrt{2c}} \int_{-T_1}^{T_1} \left( \frac{d\ell}{\sqrt{(T_1^2 - \ell^2)(A^2 + \ell^2)}} \right),
\]

\[
T_1 = \sqrt{-b + \sqrt{b^2 + \frac{4cH^2}{2b}}}, \quad H = E - W_0, \quad A^2 = \frac{b + \sqrt{b^2 + 4cH^2}}{2c}.
\]

Substituting \( t = B \cos \varphi \) we write this expression in the form:

\[
\frac{T}{2} = \sqrt{\frac{2}{c}} \frac{1}{\sqrt{T_1^2 + A^2}} \int_0^{\pi/2} \frac{dt}{\sqrt{1 - k^2 \sin^2 \varphi}} = \sqrt{\frac{2}{c}} \sqrt{\frac{T}{2T_1^2 + A^2}} K(k),
\]

where \( K(k) \) is the complete elliptic integral. As a result obtain

\[
\psi = \pi F(\Phi, k) \frac{F}{2K(k)}, \quad q = T_1 \cos \Phi
\]

where \( F(\Phi, k) \) is the elliptic integral of the first order.

### 3 Asymptotic behavior of different quantities at small energy

We are interested in the asymptotic behavior of \( T \) and the derivative \( \frac{\partial T}{\partial H} = \frac{\partial T}{\partial E} \) at \( H \to 0 \), then

\[
k = \frac{\sqrt{Hc}}{b} (1 + O(H)), \quad \frac{1}{\sqrt{T_1^2 + A^2}} = \sqrt{\frac{c}{b}} \left( 1 - \frac{Hb}{b^2} \right) + O(H^2).
\]

The smallness of \( k \) allows us to use the asymptotic formula for \( K(k) \):

\[
K(k) = \frac{\pi}{2} \left\{ 1 + \left( \frac{1}{2} \right)^2 k^2 + \left( \frac{1 \cdot 3}{2 \cdot 4} \right)^2 k^4 + \ldots \right\}.
\]

From here and \( (11) \) we have

\[
\frac{T}{2} = \frac{\pi}{\sqrt{2b}} \left( 1 - \frac{3Hc}{4b^2} \right) + O(H^2).
\]
Hence we immediately obtain the leading order in the expression for the frequency and its derivative which can be written as:

\[
\omega = \sqrt{2b + O(H^2)} = \sqrt{2U^{(2)}(1) + O(H^2)},
\]

\[
\frac{\partial \omega}{\partial E} = \frac{\partial \omega}{\partial H} = \frac{3c}{\sqrt{2ba}} + O(H) = \frac{U^{(4)}(1)}{4\sqrt{2U^{(2)}(1)}} + O(H).
\]  

(15)

Let us write the function \( q(J, \psi) \) in the terms of variables \((J, \psi)\). The error does not exceed \( O(H) \). Because of \( k \sim \sqrt{H} \) we use asymptotic formulae for \( K(k) \) (14) and \( F(\Phi, k) = \Phi + \ldots \). It results in \( \psi = \Phi + O(H) \) and \( \Phi = \varphi + O(H) \).

To calculate the Fourier coefficients (5) we expand the potential in the vicinity of \( q = 0 \):

\[
H_n = \frac{1}{\pi} \int_0^{2\pi} d\varphi \cos n\varphi \left[ U^{(2)}(1)q + U^{(3)}(1)\frac{q^2}{2!} + U^{(4)}(1)\frac{q^3}{3!} + \ldots \right].
\]

The function \( q(J, \psi) \) is equal to \( q = T_1 \cos(\varphi + O(H)) \) where \( T_1 = \sqrt{H/b} + O(H^2) \). Then we have

\[
H_2 \sim H \frac{U^{(3)}(1)}{4U^{(2)}(1)}, \quad H_3 \sim \sqrt{H^3}.
\]

From (8), (15) we have inequalities \(|\Delta \omega(I_1)| \sim \sqrt{\Delta H} \gg |\Delta \omega(I_2)| \sim \sqrt{\Delta H} \gg |\Delta \omega(I_3)| \sim \sqrt{\Delta H^3} \). It allows us to obtain expression for functions \(|K_{2,1}|, |K_{3,2}|\):

\[
|K_{2,1}| \approx \frac{\Delta \omega(I_1)}{2(\omega(I_2) - \omega(I_1))} \approx \frac{1}{\omega_1} \sqrt{\frac{1}{2} \alpha_1} H \frac{U^{(3)}(1)}{8U^{(2)}(1)},
\]

\[
|K_{3,2}| \approx \frac{\Delta \omega(I_2)}{2(\omega(I_3) - \omega(I_2))} \approx \frac{3}{\omega_1} \sqrt{\frac{1}{2} \alpha_1} H \frac{U^{(3)}(1)}{32U^{(2)}(1)} U^{(4)}(1) U^{(2)}(1).
\]  

(16)

4 Approximate action-angle variables at high energy and asymptotic behavior of different quantities

From the point of view of physics high values of energy \( E \) correspond to the fulfillment of the inequality \( E/U_0 \gg 1 \). Since the potential \( W(q) = U(1+q) + U(1-q) \) is symmetric function with respect to \( q \rightarrow -q \) it is enough to consider it at the interval \((0, 1)\). It is clear that for large values of \( E \) turning point
coordinate \( q_1 \sim 1 \). Then the leading contribution in \( V(q) \) is determined by \( U(1 - q) \). We introduce an approximate potential

\[
W_{\text{big}}(q) = \frac{1}{(1 - q)^\alpha}
\]

and action-angle variables \( J_{\text{big}}, \phi \)

\[
J_{\text{big}}(E) = \frac{2}{\pi} \int_{Q_1}^1 p_{\text{big}} dq, \quad \phi = \Omega_{\text{big}} t_{\text{big}}, \quad \Omega_{\text{big}} = \frac{\partial E}{\partial J_{\text{big}}}, \quad t_{\text{big}} = \int_{Q_1}^q \frac{dq}{p_{\text{big}}},
\]

where function \( p_{\text{big}} = \sqrt{2(E - W_{\text{big}}(q))} \), and the coordinate \( Q_1 \) is defined by the equation

\[
E = W_{\text{big}}(Q_1).
\]

From a mathematical point of view, values \( I, J_{\text{big}} \) determine the area in phase space for functions \( p, p_{\text{big}} \) respectively. Area difference can be estimated by the sum of functions

\[
|I(E) - J_{\text{big}}(E)| \leq \frac{2}{\pi} |[Q_1 - q_1] \max |p| + \int_{Q_1}^1 [p - p_{\text{big}}] dq|.
\]

Leading order of \( Q_1 - q_1 \) is determined from (17), (19) and is equal to \( Q_1 - q_1 = \frac{Q_1^{\alpha - \beta + 1}}{\beta}(1 + \frac{Q_1^{\alpha - \beta}}{\beta}) \). Since \( \max |p| \leq \sqrt{2E} \) then the first term in (20) has the following order \( (Q_1 - q_1)\sqrt{E} \sim \frac{1}{E^{1/2 + (1 - \beta)/\alpha}} \). The integral term in (20) is equal to

\[
\int_{Q_1}^1 \left| \int_{Q_1}^1 \frac{p_{\text{big}} - W}{p + p_{\text{big}}} dq \right| \sim \int_{Q_1}^1 \left| \frac{1}{p_{\text{big}}} dq \right| \sim Q_1^{1 - \beta + \alpha/2} \sim \frac{1}{E^{1/2 + (1 - \beta)/\alpha}}.
\]

Hence

\[
I(E) - J_{\text{big}}(E) \sim \frac{1}{E^{1/2 + (1 - \beta)/\alpha}}.
\]

on condition that \( \alpha > 2(\beta - 1) \) which provides a decrease in the right side of (21). Differentiation (21) with respect to \( E \) results in relations for the frequencies corresponding to the action and their derivatives:

\[
\omega E - \Omega_{\text{big}}(E) \sim \frac{1}{E^{3/2 + (1 - \beta)/\alpha}}, \quad \frac{\partial \omega}{\partial E} - \frac{\partial \Omega_{\text{big}}}{\partial E} \sim \frac{1}{E^{3/2 + (1 - \beta)/\alpha}}.
\]
The difference between the phases $\phi$ and $\phi$ is written in the form:

$$|\phi - \phi| \leq |\omega - \Omega_{big}|t_{big} + \omega|t - t_{big}| \sim \frac{t_{big}}{E^{3/2+(1-\beta)/\alpha}} + \omega|\omega - \Omega_{big}|.$$ 

For high energy frequency $\omega \sim t_{big} \sim \sqrt{E}$ then from here and (22) we have

$$\varphi - \phi \sim \frac{1}{E^{1+(1-\beta)/\alpha}} \to 0.$$ \hfill (23)

Let us transform from phase to phase in the integral (5) with accuracy (23) and use the equality $q(\phi + \pi, J_{big}) = Q_2 - q(\phi, J_{big})$. Since $2 = Q_2 + Q_1$ we rewrite (5) in the following form:

$$H_n = \frac{1}{2} \int_{Q_1}^{Q_2} dq \left[U^{(1)}(2 - q) + U^{(1)}(Q_1 + q)(-1)^n\right] \cos \frac{\pi n}{Q_2 - Q_1} q.$$

A leading term with respect to $E$ is determined by means of integration:

$$H_n = \frac{1}{2} \left[-U(L - q) + U(Q_1 + q)(-1)^n\right] \cos \left. \frac{\pi n}{Q_2 - Q_1} q \right|_{Q_1}^{Q_2} - \frac{1}{2} \frac{\pi}{Q_2 - Q_1} \int_{Q_1}^{Q_2} dq \left[U(L - q) - U(Q_1 + q)(-1)^n\right] \sin \frac{\pi n}{Q_2 - Q_1} q. \hfill (24)$$

The outside terms have a singular behavior with respect to $E$ since

$$\frac{(-1)^n}{2} \left[-U(Q_1) - U(2Q_1)\right] = -\frac{(-1)^n}{2} \frac{1}{Q_1^\alpha} [1 + 1/2^\alpha] + \frac{Q}{Q_1^\beta} = -E \frac{(-1)^n}{2} [1 + 1/2^\alpha] + \frac{Q}{Q_1^\beta}.$$ 

The integral in (24) is smaller than these terms then the Fourier coefficient is equal to

$$H_n = -E \frac{(-1)^n}{2} [1 + 1/2^\alpha] + \ldots \hfill (25)$$

From (9), (25) we obtain expression for functions $K_{n,n-1}$:

$$K_{n,n-1} = \sqrt{\frac{\alpha_1}{2}} (1 + 1/2^\alpha)(n - 1)/2.$$ 

The parameter $\alpha = 12$ for the Lennard-Jones potential then we obtain $K_{2,1} = 1.5 \sqrt{\alpha_1/2}$, $K_{3,2} = 2.5 \sqrt{\alpha_1/2}$. 

5 Comparison with numerical results for $K_{2,1}(q_0)$

The function $K_{2,1}(q_0)$ was defined numerically (exact) and calculated (asympt) in accordance with formula (16). Its behavior depending on the initial position of the resonance trajectory is presented in Fig.1 (exact). From here it is seen that formula (16) is a good approximation for $K_{2,1}(q_0)$ as for small as high energies.

![Graph of the function $K_{2,1}(q_0)$](image)

Fig. 1. Graph of the function $K_{2,1}(q_0)$ defined numerically (exact) and calculated (asympt) in accordance with formula (16).

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