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Numerical Simulation of the Ground-state of Elastic-periodic Chain of Atoms in Periodic Potential of Arbitrary Shape

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An elastic periodic chain of atoms in periodic potential has been considered. Numerical simulations revealed the existence of stepwise behavior of the ground state graph near the origin. Such behavior is not observed in the continuous medium approximation. The step height is equal to one-half the classical frequency.

Keywords: Frenkel-Kontorova model, periods incommensurate, discrete finite chain.

The Hooke model describes a one-dimensional elastic periodic chain of atoms. Extended Hooke model (EH model) describes an elastic periodic chain of atoms in periodic potential. The potential period and amplitude are taken to be arbitrary.

Extended Hooke model has been extensively studied [1–5] but those studies were limited to continuous medium approximation (string limit). In this approximation the discrete variable n is replaced by x and the ground state is determined with the use of integral-differential method. Our interest is in testing numerically the string limit results.

Consider an elastic chain of atoms with a period $M+\delta$ in the potential $V(x)$ with period 1. In the framework of the EH model potential energy is

$$U=\sum_{n=0}^{N}\left[\frac{1}{2}(u_{n+1}-u_n)^2+V(Mn+\delta+u_n)\right], \qquad V(x+1)=V(x), M=0,1,..., \tag{1}$$

where u_n is displacement of n-th atom from the initial equilibrium position.

The change $\varphi_n=u_n+n\delta$ [1] results in the following expression for potential energy:

$$U=\sum_{n=0}^{N-1}\left[\frac{1}{2}(\varphi_{n+1}-\varphi_n)^2+V(\varphi_n)\right]+V(\varphi_N)-\delta(\varphi_N-\varphi_0)+\frac{\delta^2}{2}N. \tag{2}$$

The equilibrium positions of the atoms in the EH model are exactly defined by the boundary value φ_N and by the system of equations

$$\begin{gathered} u_N-u_{N-1}-\delta+V'(\varphi_N)=0,\\ 2\varphi_n-\varphi_{n+1}-\phi_{n-1}+V'(\varphi_n)=0,\quad 0\leqslant n\leqslant N. \end{gathered} \tag{3}$$

System (3) has an infinite number of solutions because the potential $V(x)$ is periodical one. These solutions differ only by the values of φ_N. Numerical experiments with different values

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of the EH model parameters were conducted. We sought the solution of equation (3) with a minimum of (7) with respect to φ_N at $\varphi_N = \Phi_N$.

Let us compare the results obtained with the use of the EH model and the string limit results.

The main distinction between the EH model and the Hooke model is in stepwise character of the chain tensile behavior which depends on the force applied to the end of chain. Chain can be stretched by an arbitrarily weak force in the Hooke model. There is a force threshold in the EH model. If the force is below of this threshold then it is energetically favorable for the chain atoms to stay in their potential wells. Let us put the coefficient of chain elasticity equal to 1. The force threshold is denoted as δ_c. In the string limit the value of δ_c can be found from equation

$$\delta_c = \int_0^1 \sqrt{2(V(x) - V_{\min})}dx, \tag{4}$$

The qualitative behavior of the ground state graph in the EH model is shown in Fig. 1.

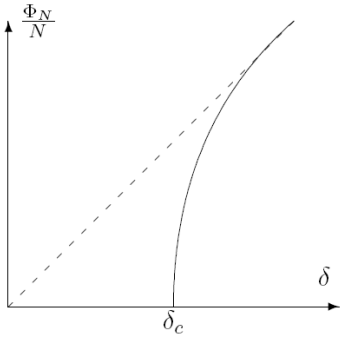

Fig. 1. The behavior of the ground state graph in the EH model

Near some rational values of $\delta = \dfrac{m}{n}$ the chain is also not stretched. The size of region of "nonstretching" dependent heavily on n and also on the number of potential harmonics. For a single harmonic potential and $\delta = \dfrac{1}{2}$ the step size is $\delta_{c,2} = \delta_c^2$ [1]. It was shown in the case of a rectangular potential that step dimensions are significantly larger than δ_c^2 near rational values [2]. The step dimensions are close to δ_c, $\delta_{c,n} \leqslant \dfrac{\delta_c}{\sqrt{n}}$.

The EH model includes two parameters N and $R = \dfrac{1}{\delta_c}$ is the size of dislocation. The case $N < R$ qualitatively differs from the case $N > R$. This is confirmed by numerical experiments. Two potentials were used in numerical experiments: single-mode potential $V(\varphi) = -V_0 \cos 2\pi\varphi$ and double-mode potential $V(\varphi) = -0.64\, V_0(\cos 2\pi\varphi + \cos 4\pi\varphi)$. For each potential δ_c is determined from equation (4):

$$\begin{aligned} &\delta_c^{(1)} = \frac{4}{\pi}\sqrt{V_0} \approx 1.272\sqrt{V_0}, \\ &\delta_c^{(2)} = \int_0^1 \sqrt{1.28V_0(3 - 2\cos^2 2\pi\varphi - \cos 2\pi\varphi)}d\varphi. \\ &\delta_c^{(2)} \approx 1.506\sqrt{V_0} \end{aligned} \tag{5}$$

Numerical simulations show that potential energy (7) has a large number of very narrow with respect to φ_N local minima. For example, in the case of double-mode potential and $N = 12$, $V_0 = 0.04$ the analysis of the ground state requires increment $h = 10^{-10}$ in the value of φ_N. Full

analysis of the EH model with basic values of its parameters requires more than 10^{30} arithmetic operations. We have restricted ourselves to selected calculations which allow us to qualitatively plot the ground state graph (Fig. 2). The results obtained with the use of the EH model considerably differ from the solutions based on the string approximation (Fig. 1).

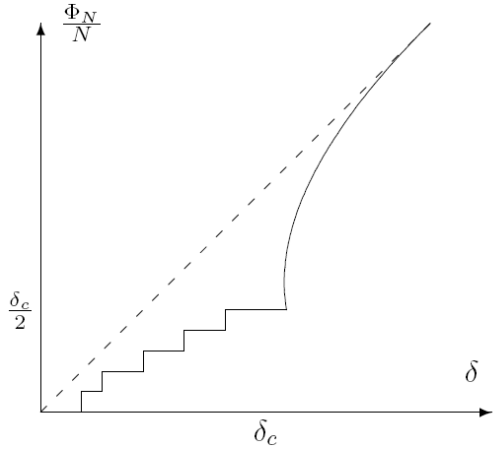

Fig. 2. Graph of the ground state in the EH mode

Our numerical results confirm only in part the previously obtained results [1–5] and the values of δ_c given in (5). In the range of incommensurate phase ($\delta > \delta_c$) chain atoms quickly change their positions as δ increases. Steps dimensions near rational values of δ are also within the previously predicted range [1, 2].

The main distinction between the exact solution and the string approximation results is in the region of commensurate phase ($|\delta| < \delta_c$).

It was believed that $\Phi_N \equiv 0$ in the range $|\delta| < \delta_c$. In fact, in this range the behavior of the graph $\Phi_N - \delta$ has a stepwise form with the step height is $\dfrac{N\delta_c}{2}$ (Fig. 3). It is easy to see that

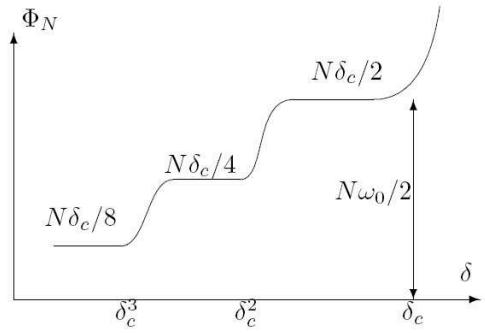

Fig. 3. Graph of (δ, Φ_N)

in the continuous limit the stationary equation of the EH model (3) coincides with the equation of motion of classical particle. Space-time coincides with Euclidean metric and the following expressions hold for potential $V(x)$:

$$\varphi''_{xx} = V'_{\varphi}(\varphi),\ x''_{tt} = V'_x(x) \tag{6}$$

The action of classical particle S with energy E is expressed in pseudo-Euclidean space-time as [6, 7]:

$$S = \int \sqrt{2(V(x) - E)}dx \tag{7}$$

Comparing (4) and (7), we conclude that δ_c coincides with the minimum of action S which is called the "classical frequency ω_0". The step height $\frac{N\delta_c}{2}$ coincides with vacuum energy of a particle in Euclidean space-time $\frac{N\omega_0}{2}$. That is why this stepwise form can be given the name "vacuum form".

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Численное моделирование основного состояния упруго-периодической цепочки атомов в периодическом потенциале произвольной формы

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Численным моделированием обнаружена лестница на начальном отрезке графика основного состояния модели упруго-периодической цепочки атомов в периодическом потенциале (РмГ-модель), отсутствующая в приближении сплошной среды. Высота лестницы равна половине классической частоты.

Ключевые слова: модель Френкеля-Конторовой, несоразмерность периодов, дискретная конечная цепочка.