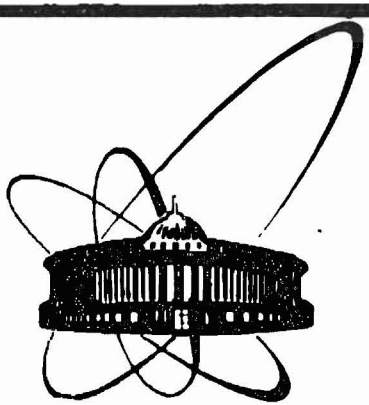

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E17-88-881

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THE HEAT CAPACITY OF THE ONE-DIMENSIONAL MODEL OF QUASIPERIODIC BINARY ALLOY

Submitted to "International Journal of Modern Physics B"

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1988

1. Introduction

Recently, the properties of the electronic and vibrational spectrum of the dynamic models of one - dimensional quasicrystals (1D QC) [1,2] are the subject of extensive studies [3,13].

So far, various thermodynamic properties of these systems having the singular continuous spectrum of elementary excitations [4,6,7] have not been investigated in detail.

In this paper we report the numerical results concerning the temperature dependence of the heat capacity C of the one-dimensional Fibonacci-type binary alloy (1D FBA) [10].

The harmonic model describing the vibrational motions of atoms is used and the next-nearest-neighbour interactions of atoms are taken into account.

The spectrum of the 1D FBA containing $F_{19}=4181$ and $F_{21}=10946$ atoms is obtained numerically and used for the calculation of the temperature dependencies of the heat capacity C in the wide range of $T_{RED}=k_BT/E_{max}$,where E_{max} is a maximal eigenenergy of the system.

Moreover, the dependence of the results on the variations of model parameters is studied in detail.

The paper is organized as follows. The specification of the investigeted model in Sec.2 is presented. Sec.3 contains the basic equations. The numerical results and concluding remarks are given in Sec.4.

2. Specification of the model

Let us briefly specify the 1D FBA model considered in this paper.

The quasilattice (QL) of the one-dimensional Fibonacci-type quasicrystal (1D FQC) [1,2] is defined by the set of points $\{x_n\}$ given by

$$x_n = n + \beta + [\, n/\tau + \alpha \,]/\tau \,, \qquad (1)$$

where α , β are the real numbers, τ is a golden ratio equal to $(1 + \sqrt{5})/2$ and $[y]$ denotes the integer part of y. We decorate 1D QL placing two types of atoms in the middle of the points given by (1) (with $\alpha=\beta=0$), i.e. the equilibrium position of n-th atom having the mass

$$m_n = m_o(1 + q([(n+1)/\tau]-[n/\tau])) \,, \qquad (2)$$

is

$$l_n = (x_{n+1}+x_n)/2 \,, \qquad (3)$$

where $q=z/\tau$ is the so-called parameter of quasiperiodicity.

In this chain (see Fig.1) we have: (1) two types of nearest-neighbour (NN) spring constants k_{HL} and k_{HH} ; (2) three types of next-nearest-neighbour (NNN) spring constants g_{HH} , g_{LH} and g_{LL}.

In this paper the 1D harmonic binary chain with quasiperiodic distribution of masses but constant isotropic forces

$$k_{HL}=k_{HH}=k_o \qquad (4a)$$

$$g_{HH}=g_{LH}=g_{LL}=g_o \qquad (4b).$$

is studied.

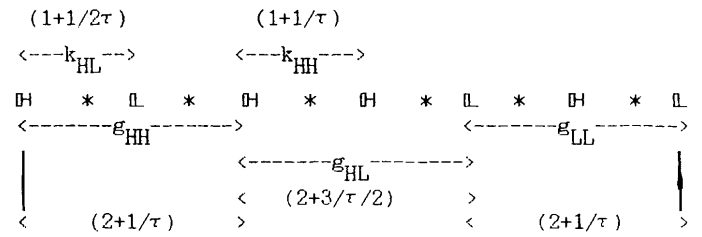

Fig.1. The harmonic interactions of nearest-neighbour (k_{HL} and k_{HH}) and next-nearest-neighbour (g_{HH}, g_{HL} and g_{LL}) atoms; the asterisks (*) indicate the points of 1D QL, the letters H and L denote the atoms whose masses are $m_o(1+q)$ and m_o , respectively; in the parenthesis the dimensionless distances between atoms are given.

Notice, that (2) defines the binary quasiperiodic sequence the properties of which has extensively been studied recently by Aviram [14,15].

3. Basic equations

The quantum-mechanical equation of motion of the system under consideration is

$$\left\{ -\sum_{i=1}^{N} \frac{\hbar^2}{2 m_i} \frac{d^2}{d u_i^2} + \frac{1}{2} \sum_{i=1}^{N} k_{i,i+1} (u_i - u_{i+1})^2 \right.$$

$$\left. + \frac{1}{2} \sum_{i=1}^{N} g_{i,i+2} (u_i - u_{i+2})^2 - E \right\} \Psi = 0 \qquad (5)$$

The Schroedinger equation (5) can be diagonalized by the normal coordinate transformation (NCT) $\vec{u}=\mathbb{W}\ \vec{Q}$ which also diagonalizes the classical equations of motion (see below) [16].

Using this NCT the equation (5) can be decomposed into N independent equations for the linear harmonic oscillators

$$\left\{ -\frac{\hbar^2}{2}\frac{d^2}{dQ_i^2} + \frac{1}{2}\omega_i^2 Q_i^2 - E_i \right\} \phi_i(Q_i) = 0 \qquad (6)$$

and the total energy of the chain consisting of N atoms is

$$E = \sum_{i=1}^{N} \hbar\omega_i \left(n_i + 1/2 \right) , \quad n_i = 1,2,3,\ldots \qquad (7)$$

The harmonic frequencies ω_i appearing in (6) and (7) can be obtained from the classical system of equations [16]

$$m_i \frac{d^2 u_i}{dt^2} = k_{i,i-1}(u_{i-1} - u_i) + k_{i,i+1}(u_{i+1} - u_i)$$
$$+ g_{i,i-2}\left(u_{i-2} - u_i \right) + g_{i,i+2}\left(u_{i+2} - u_i \right) \qquad (8)$$
$$i = 1,2,\ldots,N .$$

Introducing mass dependent variables $q_i=\sqrt{m_i}\,u_i$, $i=1,2,..N$ and the notion of normal modes $q_i(t)=q_i^0 \exp(i\omega t)$ the classical system of equations takes the form

$$\Omega^2 q_i = \alpha_i q_i + \beta_{i-1} q_{i-1} + \beta_{i+1} q_{i+1}$$
$$+ \gamma_{i-2} q_{i-2} + \gamma_{i+2} q_{i+2} \qquad (9)$$
$$i = 1,2\ldots N ,$$

where the dimensionless eigenfrequencies Ω and the strength of the next-nearest neighbour interactions are given by $\Omega^2 = m_o\omega_o^2/k_o$ and $h=g_o/k_o$, respectively and

$$\alpha_i = 2\frac{m_o}{m_i}\left(1 + h \right) \qquad (10)$$

$$\beta_{i+1} = -\frac{m_o}{\sqrt{m_i\, m_{i+1}}} \qquad (11)$$

$$\gamma_{i+2} = -h\frac{m_o}{\sqrt{m_i\, m_{i+2}}} \qquad (12)$$

The harmonic frequencies Ω_i are the eigenvalues of the N*N symmetric band matrix $\mathbb{D}$ of width five if the free boundary conditions are applied ($k_{i,j}=g_{i,j}=0$ if i or j lie outside the range 1 to N inclusive)

$$\mathbb{D}\, q = \Omega^2 q . \qquad (13)$$

where

$$\mathbb{D} = \begin{bmatrix} \alpha_1 & \beta_2 & \gamma_3 & & & & & \\ \beta_2 & \alpha_2 & \beta_3 & \gamma_4 & & & & \\ \gamma_3 & \beta_3 & \alpha_3 & \beta_4 & \gamma_5 & & & \\ & \gamma_4 & \beta_4 & \alpha_4 & \beta_5 & \gamma_6 & & \\ & & \ddots & \ddots & \ddots & \ddots & & \\ & & & \ddots & \ddots & \ddots & & \\ & & & & \gamma_{N-2} & \beta_{N-2} & \alpha_{N-2} & \beta_{N-1} & \gamma_N \\ & & & & & \alpha_{N-1} & \beta_{N-1} & \alpha_{N-1} & \beta_N \\ & & & & & & \gamma_N & \beta_N & \alpha_N \end{bmatrix} \qquad (14)$$

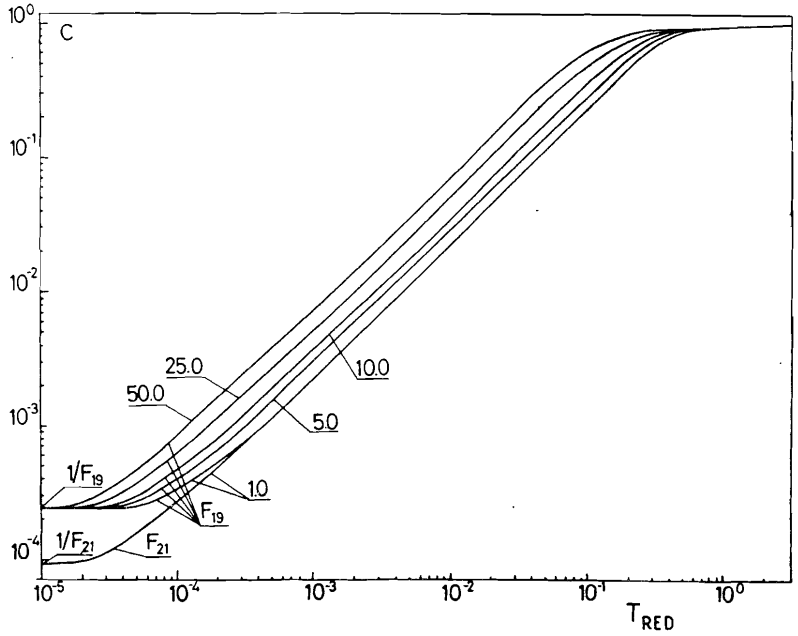

Fig.2. The heat capacity $\mathbb{C}$ plotted as a function of the reduced temperature T_{RED} for the indicated values of z (1.0,5.0,10.0,25.0,50.0); h=0 and the number of atoms N is equal to F_{19}; for z=1.0 the results obtained for $N=F_{19}$ and F_{21} are presented,too.

We have diagonalized numerically the dynamic matrix $\mathbb{D}$ using EISPACK routines for the number of atoms $N=F_{19}$ and $N=F_{21}$, where F_{19}= 4181 and F_{21}= 10946 are the Fibonacci numbers.

The obtained eigenvalues Ω_i have been used further to calculate of the heat capacity

$$\mathbb{C}(T_{RED})=\frac{C(T_{RED})}{N\ k_B}=\sum_{i=1}^{N}\frac{\nu_i}{N}\left(\frac{\varepsilon_i/T_{RED}}{1-\nu_i}\right)^2, \quad (15)$$

where $\varepsilon_i=\Omega_i/\Omega_{max}$, $\nu_i=\exp(-\varepsilon_i/T_{RED})$, $T_{RED}=k_BT/E_{max}$ and $E_{max}=h\,\Omega_{max}$ where Ω_{max} denotes the maximal value of Ω_i.

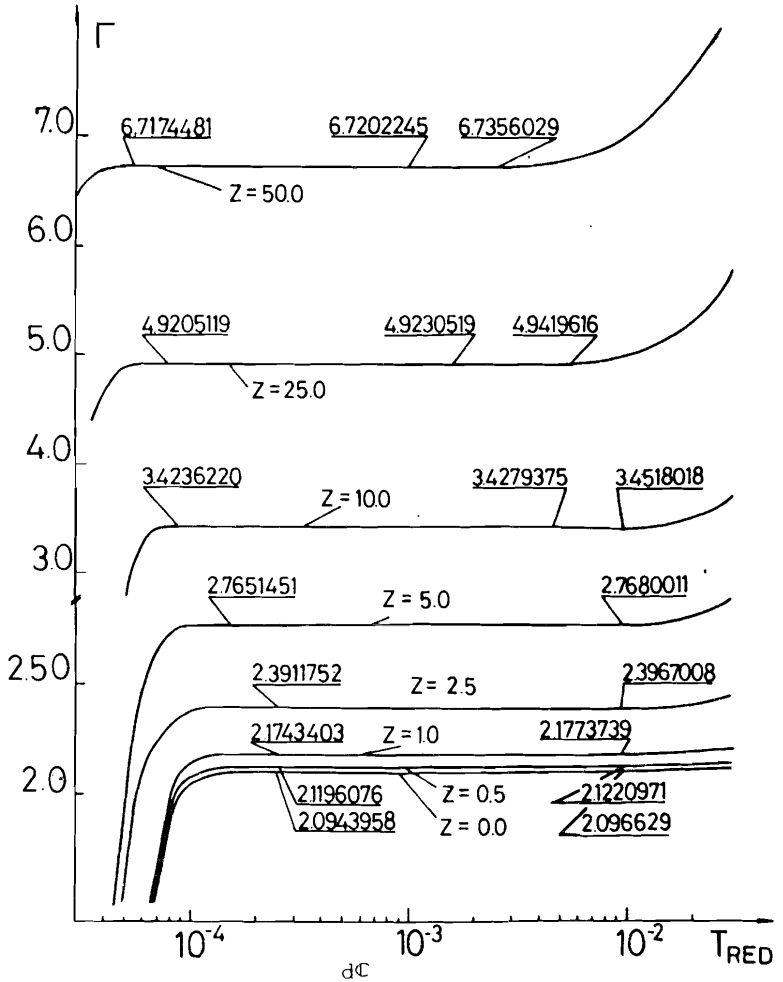

Fig.3.The derivative $\Gamma=\frac{d\mathbb{C}}{d'T_{RED}}$ plotted as a function of T_{RED}.

4. Numerical results and discussion

The temperature dependencies of the heat capacity $\mathbb{C}$ and the difference of $\mathbb{C}$ with respect to T_{RED} in Figs.2÷5 are presented.

From the results of our computer simulations the following facts and trends are immediately apparent.

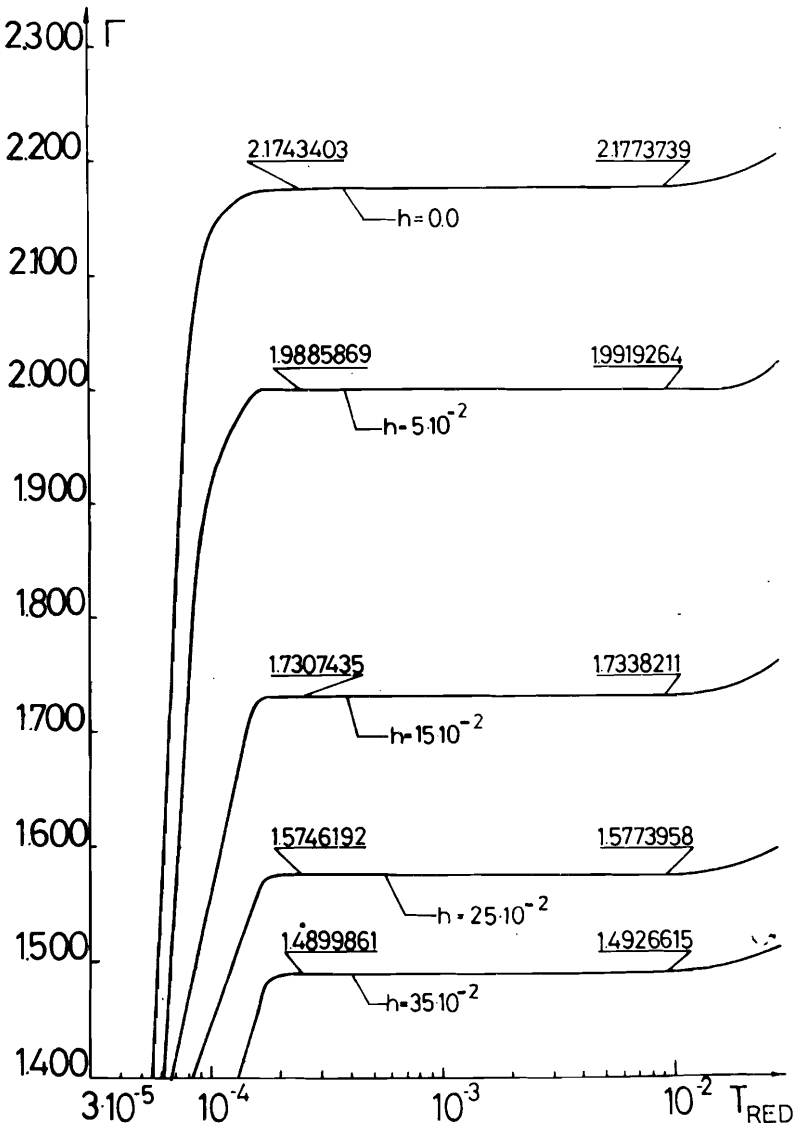

Fig.4. The same as in Fig.3 for $N=F_{19}$, $z=1.0$ and h is equal to 0.0, 0.05, 0.15, 0.25 and 0.35.

1. At sufficiently low temperatures the heat capacity $\mathbb{C}$ is a linear function of the reduced temperature, i.e. there exists the magnitude of T_{RED} below which

$$\mathbb{C}(T_{RED}) = \Gamma(z,h)\, T_{RED}, \qquad (16)$$

where Γ is a constant depending on model parameters z and h (cf. Figs. 2-5).

The plots in Figs. 3-5 show that Γ is almost independent of temperature at $T_{RED} \lesssim 10^{-2}$. Moreover, in Figs. 3÷5 the beginning (Γ_B) and the end (Γ_E) of each plateau is indicated by the calculated values of Γ. Notice that in the region of each plateau the parameter

$$\vartheta = 2\,(\Gamma_E - \Gamma_B)\,/\,(\Gamma_E + \Gamma_B) \qquad (17)$$

describing the relative slopes of Γ is less than 0.3 %.

2. At high temperatures, ($T_{RED} \gtrsim 1$) the heat capacity $\mathbb{C}$ approaches the value given by Dulong-Peti law.

3. The variation of models parameter z and h leads to the quantitative changes of $\mathbb{C}$ and Γ. The heat capacity increases with z (cf. Figs. 2,3) and Γ diminishes with increasing of h (cf. Fig. 4).

We have studied also the finite size effects in $\mathbb{C}$ and Γ. Comparison of the calculated results for different numbers of atoms N in the chain in Figs. 2,5 is shown. As has been expected, the linear dependence of $\mathbb{C}$ on T_{RED} is observed in the wider low-temperature region for the larger values of N. These results confirm our first conclusion given above.

Finally, let us interpret the obtained numerical results in terms of the integrated density of states $G(\varepsilon_i^2)$ [17].

In the framework of the studied model we find that:

A1. In the optical region of vibrational spectrum (VS) $G(\varepsilon_i^2)$ exhibits the self-similar structure which is characteristic feature of the singular continuous spectrum.

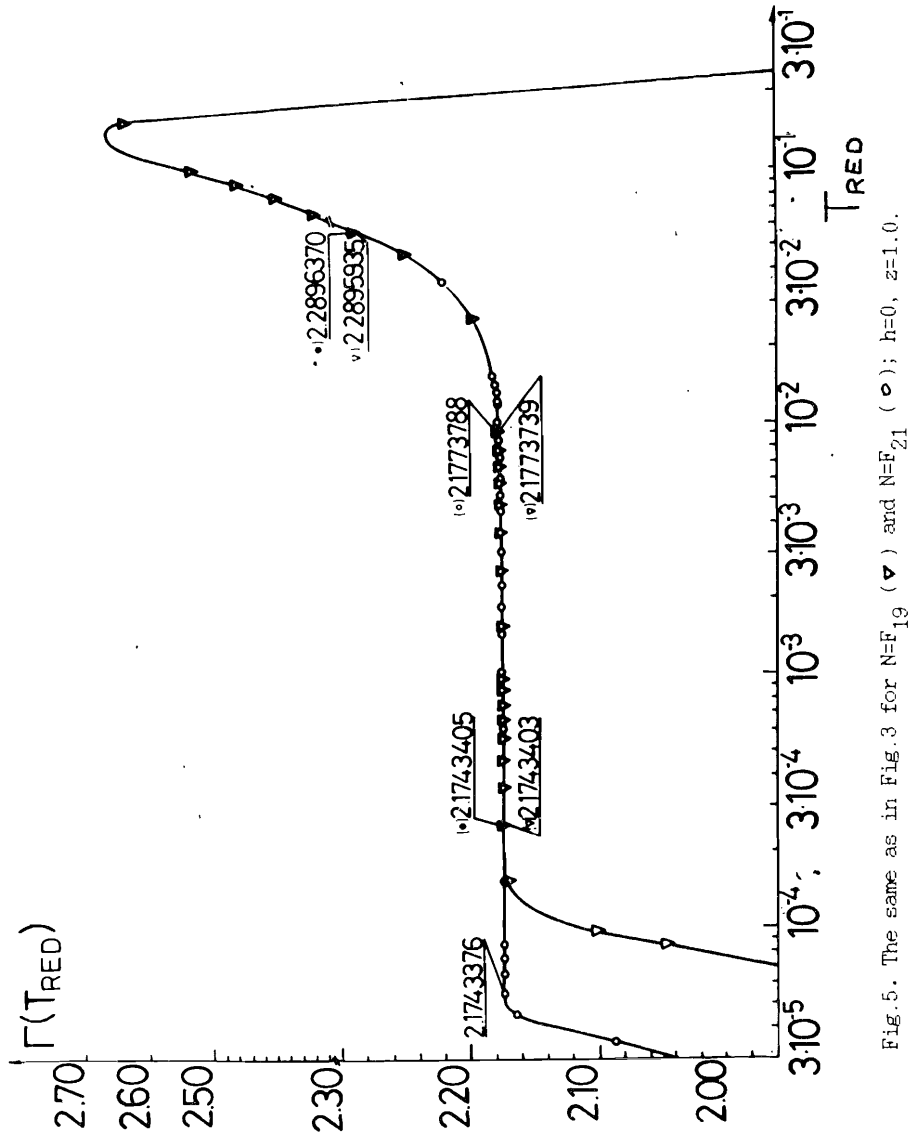

Fig.5. The same as in Fig.3 for $N=F_{19}$ (▽) and $N=F_{21}$ (○); h=0, z=1.0.

A2. In acoustic region of VS the number of gaps and their sizes tend to zero [4,9] and $G(\varepsilon_i^2)$ looks like as that of the ideal periodic chain

$$G(\varepsilon_i^2) = G(z,h)\,\varepsilon_i^2 , \qquad (18)$$

where G(z,h) is a constant depending on the model parameters. In addition, we find that G(z,h) increases with z and diminishes if the parameter h is growing up [17].

For these reasons we can conclude that the obtained temperature dependencies of the heat capacity of the studied harmonic model of 1D FBA behave identically as for the periodic chain [18].

Acknowledgments

I would like to thank • N.M.Plakida for valuable discussions. I am grateful to T.Paszkiewicz for useful comments. J.Malek helped with some of the numerical work. Computations were done at the Laboratory of Computing Techniques and Automation of the Joint Institute for Nuclear Research.

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Received by Publishing Department
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Салейда В. E17-88-881

Теплоемкость в одномерной модели
квазипериодического бинарного сплава

Исследуется температурная зависимость теплоемкости гармонической модели квазипериодического бинарного сплава. Нумерически вычислены колебательные спектры и теплоемкость С цепочки, содержащей F_{19} = 4191 и F_{21} = 10946 атомов. В области низких температур ($T_{red} < 10^{-2}$) $C(T_{red})=A*T_{red}$, где $T_{red} = k_B*T/E_{max}$, A и E_{max} обозначают, соответственно, константу зависящую от параметров модели и максимальное собственное значение динамической матрицы.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна 1988

Salejda B. E17-88-881

The Heat Capacity of the One-Dimensional
Model of Quasiperiodic Binary Alloy

The temperature dependence of the heat capacity C of the harmonic model of quasiperiodic binary chain of atoms is studied numerically. It is shown that $C(T_{red})=A*T_{red}$ at $T_{red} = k_B\ T/E_{max} \lesssim 10^{-2}$, where A is a constant depending on model parameters and E_{max} denotes a maximal eigenenergy of the dynamic matrix. At high temperatures C approaches the Dulong-Peti limit.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

Proprint of the Joint Institute for Nuclear Research. Dubna 1988