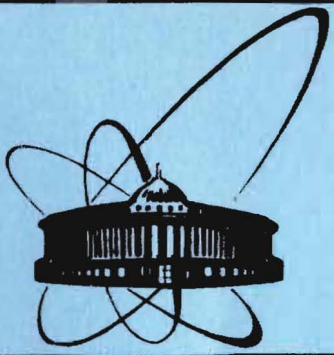

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A NOTE ON THE ENERGY LEVELS OF A SIMPLE MODEL OF STRUCTURAL PHASE TRANSITIONS - ONE DIMENSIONAL CASE

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Krumhansl and Schrieffer (1975) (KS) in their pioneering work have studied the thermodynamic and some dynamic properties of the one-dimensional model system

$$H = \sum_{l}\left\{\frac{P_l^2}{2M} - \frac{A}{2}Q_l^2 + \frac{B}{4}Q_l^4\right\} + \frac{1}{4}\sum_{ll_1}\Phi_{ll_1}\left(Q_l - Q_{l_1}\right)^2, \quad (1)$$

whose various modifications were used to study the phase transitions (see, e.g., Bruce and Cowley (1980)). In the classical approximation, by using the transfer integral matrix (TIM) method, they calculated the energy levels of system (1) in the continuum representation

$$H = \int_0^L \frac{dx}{l}\left\{\frac{P^2(x)}{2M} - \frac{A}{2}Q^2(x) + \frac{B}{4}Q^4(x) + \frac{1}{2}Mc_0^2\left(\frac{dQ}{dx}\right)^2\right\}, \quad (2)$$

where l is lattice spacing, $L/l\ (= N)$ denotes the number of particles. On this basis they showed that kink and phonon excitations contribute to the energy of the lowest energy levels (in the low temperature region). They were also able to show that the presence of the central peak is associated with the motion of domain walls.

In this note we shall show how omitting all TIM procedure (see also Scalapino et al. 1972, Kac and Helfand 1963) its final equation may be immediately obtained. Then, we shall discuss the problem of calculation of energy levels in the WKB-type approximation by using path integral method (Dashen et al. 1974, Rajaraman 1975, Radosz 1985 (I)).

In the classical approximation, the partition function Z

$$Z = \int \mathcal{D}\{P\}\,\mathcal{D}\{Q\}\exp\left\{-\beta H(P,Q)\right\} \quad (3)$$

may be written in the following form (KS):

$$Z \simeq Z_P Z_Q = \left(\frac{2\pi H}{\beta h^2}\right)^{N/2} Z_Q \quad , \tag{3a}$$

where

$$Z_Q = \int dQ_0 \; K_Q(Q_0 Q_0; L) \quad , \tag{4a}$$

$$K_Q(Q_1 Q_2; L) = \int_{Q(0)=Q_1}^{Q(L)=Q_2} \mathcal{D}\{Q\} \exp\left\{ \frac{\beta}{L} \int_0^L dx \left[\frac{1}{2} M c_0^2 \left(\frac{dQ}{dx}\right)^2 - \frac{A}{2} Q^2 + \frac{B}{4} Q^4 \right] \right\} . \tag{5a}$$

Let us for a moment consider a particle with mass m moving under the influence of a double-well potential

$$V(u) = -\frac{A}{2} u^2 + \frac{B}{4} u^4 \quad . \tag{6}$$

(A and B in Eqs.(1) and (6) are chosen in such a way that H and V are measured in energy units).

Then, the expression for Z_u (see,e.g.Rajaraman1975)

$$Z_u = \mathrm{Tr}\left[\exp\left(-\frac{i}{\hbar} H T\right)\right] = \int du_0 \langle u_0 | e^{-\frac{i}{\hbar} H T} | u_0 \rangle \tag{4b}$$

$$= \sum_n e^{-\frac{i}{\hbar} E_n T} = \int du_0 \; K_u(u_0 u_0; L) \quad ,$$

where

$$K_u(u_1 u_2; T) = \int_{u(0)=u_1}^{u(T)=u_2} \mathcal{D}\{u\} \exp\left\{ \frac{i}{\hbar} \int_0^T dt \left[\frac{1}{2} m \left(\frac{du}{dt}\right)^2 + \frac{A}{2} u^2 - \frac{B}{4} u^4 \right] \right\} \tag{5b}$$

takes the same form as Z_Q (Eqs.(4a) and (5a)) under the formal transformation

$$t \to -ix \quad , \tag{6a}$$

$$T \to -iL \quad , \tag{6b}$$

$$u \to Q \quad , \tag{6c}$$

$$\hbar \to L/\beta \quad , \tag{6d}$$

$$m \to M c_0^2 \quad . \tag{6e}$$

Therefore, we may express Z_Q as

$$Z_Q = \sum_n e^{-\frac{1}{(L/\beta)} E_n L} \quad , \tag{7}$$

where E_n are energy levels of particle m calculated from the Schrödinger equation

$$\left\{ -\frac{\hbar^2}{2m} \frac{d^2}{du^2} - \frac{A}{2} u^2 + \frac{B}{4} u^4 \right\} \psi_n(u) = E_n \psi_n(u) \tag{8}$$

with the final transformation (6c-e). Under this transformation, Eq.(8) has the form of Krumhansl and Schrieffer "the effective oscillator equation", where their term S_0 is absent. Thus, in this case of the classical approximation Eq.(3a), the problem of energy levels of one space (1D)- one time model has been reduced to the problem of single-particle energy levels (Eqs.(4b) and (5b)). It is obvious that this procedure might easily be extended in the case of other 1D models where TIM method is used (Currie et al. 1980).

Although the case of a particle in a double - well potential, Eq.(6), has been widely discussed (see, e.g., Coleman 1979, Gildener and Patrascioiu 1977), the results did not seem satisfactory (I), also because only the lowest energy levels have been obtained. We show that higher energy levels, $E_n \gtrsim V_0 \equiv A^2/4B$ may be calculated (in the WKB approximation), what might be interesting in this case (1) (see Eq.(7)).

As usually (e.g., Dashen et al. 1974, Rajaraman 1975), we are interested in the semiclassical trajectories $u_{sol}(t)$ that, satisfy the following equation of motion:

$$\frac{1}{2} m \dot{u}_{sol}^2 = (E - V_0) - V(u_{sol}) . \tag{9}$$

where we have chosen the constant of integration in such a way that energy $E > 0$. It has been shown (I) that the energy levels "within" the well $E < V_0$ were found under strong condition $E_n \ll V_0$. In the case $E \gtrsim V_0$, Eq.(9) may be written in the form of the elliptic equation

$$\left(\frac{d\bar{u}}{d\bar{t}}\right)^2 = \left(1-\bar{u}^2\right)\left(k^2\bar{u}^2 - k'^2\right) , \tag{10}$$

where

$$\bar{u}^2 = \left(\sqrt{\frac{4E}{B}} + \frac{A}{B}\right)^{-1} u^2 , \tag{10a}$$

$$\bar{t}^2 = \frac{B}{m}\sqrt{\frac{4E}{B}}\, t^2 , \tag{10b}$$

$$k^2 = 1-k'^2 = \left(2\sqrt{\frac{4E}{B}}\right)^{-1}\left(\sqrt{\frac{4E}{B}} + \frac{A}{B}\right) . \tag{10c}$$

The solution of Eq.(10) is the two-periodic function (Byrd and Friedman 1971)

$$\bar{u}(\bar{t}) = cn(\bar{t},k) \tag{11}$$

with only two turning points $\bar{u} = \pm 1$. Thus, the Green function

$$G(\epsilon) = \int du_0\, K_n(u_0 u_0; \epsilon) = \sum_{paths} T_{path} \exp\left(\frac{i}{\hbar} W_{path} + i\theta_{path}\right) \tag{12}$$

is easily calculated (for a more detailed discussion see I). The energy levels, as the poles of $G(\epsilon)$, are the solutions of the following equation:

$$W(\epsilon) = \frac{4}{3}\frac{A^2}{B}\left(\frac{A}{m}\right)^{-\frac{3}{2}}\left[2k'^2 K(k) + 2E(k)\left(2-k^2-3k'^2\right)\right] = (2n+1)\pi\hbar , \tag{13}$$

where K(k) and E(k) are complete elliptic integrals (Byrd and Friedman 1971). The right-hand side of Eq.(13) takes a relatively simple

form in two limiting cases

a) $k^2 \to 1$ $\left(k'^2 \to 0\right)$, $E \sim V_0$,

b) $k^2 \to \frac{1}{2}^+$ $\left(k'^2 \to \frac{1}{2}^-\right)$, $E \gg V_0$.

The detailed analysis of Eqs.(4),(6),(10) and (13) and the results of paper I show that the properties of those semiclassical energy levels (temperature dependent!) of the system (2) are the following: in the range of low temperatures $T \ll T^*$

$$E_n^{\pm} = \sqrt{\frac{2A}{m^*}}\left\{\left(n+\frac{1}{2}\right) \pm \frac{1}{2\pi}\exp\left(-\frac{16}{3}\frac{V_0}{\sqrt{\frac{2A}{m^*}}}\right)\right\} . \tag{14}$$

where we used after KS $m^* = Mc_0^2/(kT)^2$. There are no energy levels within well $E \lesssim V_0$ in the range of higher temperatures

$$T \gtrsim T^* = \left(\frac{32}{3\pi}\right)\frac{T^* V_0}{\sqrt{A/m^*}} , \tag{15}$$

where T^* is defined by the condition

$$W(E)\big|_{k\sim 1} = \pi\hbar kT \tag{16}$$

Higher energy levels $E_n \gg V_0$ are found from Eq.(13)

$$E_n = V_0\left\{\left(n+\frac{1}{2}\right)\frac{3\pi}{8\sqrt{2}\,K\left(\frac{1}{2}\right)}\frac{\sqrt{\frac{2A}{m^*}}}{V_0}\right\}^{\frac{4}{3}} \tag{17}$$

As it follows from Eq.(17), in the high-temperature region

$$\frac{1}{2}\frac{3\pi}{8\sqrt{2}\,K\left(\frac{1}{2}\right)}\frac{\sqrt{\frac{2A}{m^*}}}{V_0} \gg 1$$

the energy of the lowest level E_0 is proportional to $T^{\frac{4}{3}}$. Detailed information concerning those energy levels $E_n \gtrsim V_0$ may be found through a numerical solution of Eq.(13). If we are interested, for example, in the correlation functions (KS, Scalapino et al.1972), then wave functions $\Psi_n(u)$ should also be found from Eq.(8).

Above considerations allow us to throw some light on some ambiguities associated with interpretation of Eq.(8) obtained within TIM

method: as it follows from Eqs.(6) the role of $\hbar$ is played by $1k_BT$ ($\hbar = 1$ - KS, $\hbar$ is proportional to T - Currie et al. 1980, although Scalapino et al. 1972 gave the proper, within their model, meaning of $\hbar$ ($= 1kT_c$)). The quantity s_0 which is absent in our Eq.(8) follows from the difference in definition of Z_U and Z_Q, where there is no any renormalization term in functional integration in Eq.(4a) (cf. Feynman and Hibbs 1969). In the thermodynamic considerations this term should be added. Combining it with $-k_BT \ln Z_P$, one obtains (KS - Eq.(38a)) $NkT \ln(\hbar\omega_0/kT)$. (KS omitted $\hbar$ in an effect of their definition of Z_P, but then they established for a set of harmonic oscillators $\hbar = 1$(!) and in an effective oscillator equation they also proposed $\hbar = 1$).

We want to emphasize two points. Firstly, there is a difference between KS (Eq.(34-1)) and our result (Eq.14) where in exponent KS have a factor 4 instead of our 16/3. Let us mention that Jona-Lasinio et al. (1981) obtained the same exponent as in Eq.(14) (in their notation) by using the method of stochastic mechanics. Secondly, as our calculations are within WKB-type approximation rather suprisingly we find an almost exact agreement between our value of T* and the numerical result of Bishop and Krumhansl (1975) $\mu_c = 0.85$, where

$$\mu_c = \frac{1}{4}\frac{T^*}{T^* V_0 \sqrt{\frac{A}{m^*}}} = \frac{1}{4}\frac{32}{3\pi} \simeq 0.85 \quad . \tag{18}$$

The analysis similar to the above presented Eqs.(9-17) would be made on the basis of Eq. (4a) and (5a) (imaginary time formalism). Although all the results in both formalisms, imaginary - and real-time, are the same we prefer the last one as there is a simple interpretation of the constant of integration in Eq.(9) as an energy, $E = 1/2\, m\dot{u}^2 + V(u)$. In the imaginary-time formalism $Q_{sol}(x)$ is of type of the elliptic function $sn(x, k)$. In the limit of small energies $E \to 0$, $k \to 1$ and $sn\, x \to \tanh x$, which is the well-known solution used in the instanton picture (e.g., Gildener and Patrascioiu 1977, Vainhstein et al. 1982 and also Krumhansl and Schrieffer 1975). As it has been pointed out in I this solution describes the motion only "under" the barrier.

Let us also point out our believing at last. The "true" levels of 1D -one time model would allow one to obtain approximate (classical approximation of the type (3a)) energy levels of 2D model

(transformation for time is of type (6)). It might be useful for a better understanding of phenomena associated with phase transition which in 2D models takes place at $T_c \neq 0$. At the moment there is much more information about the exact energy levels in sine-Gordon 1D- one time model than about energy levels in "φ^4" 1D - one time (Dashen et al. 1975). However, in our next paper we shall discuss some properties of the 2D - "φ^4" model on the basis of the results of Hammer et al. (1981).

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Радом А. E17-85-646

Энергетические уровни в простой модели структурного фазового перехода - одномерный случай

Показано, что задача нахождения конфигурационной части статистической суммы одномерной модели типа ϕ^4 сводится к квантовомеханической задаче нахождения энергетических уровней частицы, движущейся в двойной яме потенциала. Эти уровни можно найти при помощи интегралов по траекториям. Низко- и высоколежащие уровни были найдены в явной форме.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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Radosz A. E17-85-646

A Note of the Energy Levels of a Simple Model of Structural Phase Transitions - One Dimensional Case

It is shown that in the classical approximation the configurational part of the partition function Z_Q of a one-dimensional model Hamiltonian takes a particularly simple form. The problem of calculation of Z_Q is thus reduced to the problem of finding the energy levels of one particle moving under influence of the double-well potential. Higher and lower energy levels are easily found in the WKB-type approximation.

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

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