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ON THE PARTITION FUNCTION OF d+1 DIMENSIONAL KINK-BEARING SYSTEMS

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In this note which is in a sence a continuation of the earlier paper of one of us[1] we shall discuss the properties of the classical partition function of the d+1 dimensional (d+1 D) one component kink-bearing system. It will be suggested that under some conditions the thermodynamical properties of such a system are equivalent to the properties of an appropriate dD quantum system. In fact we are interested in the behaviour of the ground state of a dD system but a possible phase transition is expected to be associated with the degeneracy of this state. Thus, also the behaviour of the first excited state is interesting. We suggest two variational schemes to study the properties of the ground state of a dD system but the detailed discussion of these methods and results in a particular case of ϕ^4 model will be presented in a separate paper.

The system under consideration is defined by the following Hamiltonian:

$$H = \sum_{\ell} \left[\frac{p_{\ell}^2}{2m} + V(x_{\ell}) \right] + \frac{1}{4} \sum_{\ell \ell_1} \Phi_{\ell \ell_1} (x_{\ell} - x_{\ell_1})^2 , \qquad (1)$$

where x_{ℓ} and p_{ℓ} are canonically conjugated coordinate and momentum, respectively, of an ℓ-th atom with mass m moving under influence of a single particle potential $V(x)$ with degenerate minima (In the well-known case of ϕ^4 model $V(x) = -(A/2)x^2 + (B/4)x^4$). ℓ denotes a vector of a simple, d+1D hypercubic lattice with lattice constant a. We shall use a notation:

$$\ell = (\ell_0, \vec{\ell}) = (\ell_0, \ell_1 \dots \ell_d) , \quad \ell_i = 1 \dots N_i , \quad i = 0, 1 \dots d .$$
$$N_0 \cdot N_1 \cdot N_2 \cdot \dots N_d = N_0 N \equiv N' . \qquad (1a)$$

Let us assume the nearest neighbour interaction with strength Φ_0 between atoms along one direction

$$\Phi_{\ell' \ell''} \equiv \Phi^{\ell_0' \ell_0''}_{\vec{\ell}' \vec{\ell}''} \equiv \begin{cases} \Phi_0 \, \delta_{\vec{\ell}' \vec{\ell}''} \delta_{\ell_0' \ell_0'' \pm 1} \\ \Phi_{\vec{\ell}' \vec{\ell}''} \delta_{\ell' \ell''} \end{cases} , \qquad (2)$$

then the partition function in classical approximation $Z_{c\ell}^{(d+1)}$, takes the following form

$$Z_{c\ell}^{(d+1)} = Z_p Z_x = (2\pi\hbar)^{-N'} (2\pi m/\beta)^{\frac{N'}{2}} Z_x ,$$

$$Z_x = \int \prod_{i=1}^{N_0} d\hat{x}^i \exp(-\beta \sum_{i=1}^{N_0} [\frac{1}{2}\Phi_0(\hat{x}^{i+1} - \hat{x}^i)^2 + U(\hat{x}^i)]) , \tag{3}$$

where the notation $x_\ell = x_{(\ell_0, \vec{\ell})} \equiv x_{\vec{\ell}}^{\ell_0}$,

$$\hat{x}^i = \{ x_{\vec{\ell}}^i : (\vec{\ell} = \ell_1, \ldots, \ell_d), \quad \ell_i = 1, \ldots N_i \}, \tag{4a}$$

$$d\hat{x}^i = \prod_{\vec{\ell}} dx_{\vec{\ell}}^i , \tag{4b}$$

$$U(\hat{x}_i) = \sum_{\vec{k}} V(x_{\vec{k}}^i) + \frac{1}{4} \sum_{\vec{k}\vec{k}'} \Phi_{\vec{k}\vec{k}'}(x_{\vec{k}}^i - x_{\vec{k}'}^i)^2 , \tag{4c}$$

$$(\hat{x}^{i+1} - \hat{x}^i)^2 = \sum_{\vec{k}} (x_{\vec{k}}^{i+1} - x_{\vec{k}}^i)^2 \tag{4d}$$

is used. (There are usual periodic boundary conditions in Eq. (3), but for simplicity they have not been written explicitly). The configurational part of partition function may be written as follows

$$Z_x = \int d\hat{x}^0 K^{(N_0)}(\hat{x}^0, \hat{x}^0; L_0) , \tag{5}$$

where

$$K^{(N_0)}(\hat{x}'', \hat{x}'; L_0 = N_0 \cdot a) =$$

$$= \int \prod_{i=1}^{N_0-1} d\hat{x}^i \exp(-\frac{1}{(\frac{a}{\beta})} a \sum_{i=0}^{N_0-1} [\frac{1}{2}\Phi_0 a^2 (\frac{\hat{x}^{i+1} - \hat{x}^i}{a})^2 + U(\hat{x}^i)]) \Big|_{\hat{x}^0 = \hat{x}',\ \hat{x}^{N_0} = \hat{x}''} . \tag{5a}$$

As we are interested in a limit $N_0 \to \infty$, there appear a natural question, under what conditions we may consider $K^{(N_0)}$, (5a), as a propagator in imaginare "time" L_0 in d D system. In fact, when we consider d D system with Hamiltonian

$$\mathcal{H} = \sum_{\vec{k}} [\frac{p_{\vec{k}}^2}{2\mu} + v(s_{\vec{k}})] + \frac{1}{4} \sum_{\vec{k}'\vec{k}''} \Phi_{\vec{k}'\vec{k}''}(s_{\vec{k}'} - s_{\vec{k}''})^2 , \tag{6}$$

then

$$Z_q^{(d)} = \mathrm{Tr}[\exp(-\tilde{\beta}\mathcal{H})] = \sum_n \exp(-\tilde{\beta}E_n) =$$

$$= \int d\hat{s}^0 \int_{\hat{s}(0)=\hat{s}^0}^{\hat{s}(\tau_0)=\hat{s}^0} D[\hat{s}(\tau)] \exp(-(1/\tilde{\hbar}) \int_0^{\tau_0} d\tau \{ \sum_{\vec{k}} [\frac{1}{2}\mu \dot{s}_{\vec{k}}^2 + \nu(s_{\vec{k}})] +$$

$$\frac{1}{4} \sum_{\vec{k}\vec{k}'} \phi_{\vec{k}\vec{k}'}(s_{\vec{k}} - s_{\vec{k}'})^2 \}) = \lim_{M \to \infty} \int d\hat{s}^0 K^{(M)}(\hat{s}^0, \hat{s}^0; \tau_0 = \tilde{\beta}\tilde{\hbar}) , \tag{7a}$$

$$K^{(M)}(\hat{s}^0, \hat{s}^0; \tau_0 = \tilde{\beta}\tilde{h}) =$$

$$= (\frac{2\pi\tilde{h}\tau_0}{\mu M})^{-N/2} \int \prod_{i=1}^{M-1} \frac{d\hat{s}_i}{(\frac{2\pi\tilde{h}\tau_0}{\mu M})^{N/2}} \exp\{ -\frac{1}{\tilde{h}}(\frac{\tau_0}{M}) \sum_{i=0}^{M-1} [\frac{1}{2}\mu(\frac{\hat{s}^{i+1} - \hat{s}^i}{a})^2 + u(\hat{s}^i)]\} . \tag{7b}$$

In the above formulae (7a) and (7b), notation (4) is used and periodic boundary conditions for d D lattice with $N = N_1 \cdot N_2 \cdot \ldots N_d$ atoms, are taken into account. Propagator $K^{(N_0)}(\hat{s}'', \hat{s}'; \tau_0)$, (7a) transforms into $(2\pi/\beta\Phi_0)^{-N_0 N/2} K^{(N_0)}(\hat{x}'', \hat{x}'; L_0)$, (5a), under the transformation

$$\hat{s} \to \hat{x} , \tag{8a}$$

$$\tau_0 \to L_0 , \tag{8b}$$

$$(\tau_0/N_0) \to a , \tag{8c}$$

$$\tilde{h} \to (a/\beta), \quad \text{then} \quad \tilde{\beta} \to \beta N_0 , \tag{8d}$$

$$\mu \to \Phi_0 a^2 , \tag{8e}$$

$$u \to U \Leftrightarrow v(x) = V(x) , \quad \phi_{\vec{k}\vec{k}'} = \Phi_{\vec{k}\vec{k}'} . \tag{8f}$$

We expect, that when smooth enough trajectories give dominating contribution into expression (5a) then in the limit of large N_0 the approximate equality takes place

$$Z_x \approx (2\pi/\beta\Phi_0)^{N_0 N/2} \sum_n \exp(-\beta N_0 \epsilon_n) , \tag{9}$$

where ϵ_n are determined by the eigenvalues of a Schrödinger equation for d D system

$$\{\sum_{\vec{k}}[-\frac{\tilde{\hbar}^2}{2\mu}\frac{d^2}{ds^2_{\vec{k}}}+v(s_{\vec{k}})]+\frac{1}{4}\sum_{\vec{k}\vec{k}'}\phi_{\vec{k}\vec{k}'}(s_{\vec{k}}-s_{\vec{k}'})^2\}\Psi_n(\{s_{\vec{k}}\})=E_n\Psi_n(\{s_{\vec{k}}\}),$$

$$\epsilon_n = E_n \Big|_{\frac{\tilde{\hbar}^2}{2\mu}=(2\beta\Phi_0)^{-1}} . \tag{10}$$

The interaction term in Eq. (4c)

$$\sum_{\vec{k}\vec{k}'}\Phi_{\vec{k}\vec{k}'}(s_{\vec{k}}-s_{\vec{k}'})^2$$

is insensitive to an homogeneous displacement of all particles in a "transverse" d D hyperplane of d + 1 D hypercubic lattice. Therefore, the contribution of the trajectories with small changes between i-th and i + 1 -th configuration

$$(\hat{x}_{i+1}-\hat{x}_i)^2 \ll N x_0^2 , \tag{11}$$

will be most significant when the relation between "kinetic" energy term, $(1/2)\,\Phi_0(\hat{x}^{i+1}-\hat{x}^i)^2$, and (single particle) potential energy term, $\sum_{\vec{k}} V(x^i_{\vec{k}})$, will prefer rather small changes of coordinates than large "jumps" (between minima of V(x)),

$$(1/2)\,\Phi_0 x_0^2 \gg V_0 . \tag{12}$$

In the above inequalities (11) and (12), x_0 and V_0 denote the distance and energy barrier, respectively, between neighbouring minima of V(x) . In the case of double well potential

$$V_0 = A^2/4B , \quad x_0 = 2\sqrt{A/B} \tag{13a}$$

and the condition (12) denotes a well-known displacive limit (see [2])

$$\Phi_0 \gg (1/8)\,A . \tag{13b}$$

Therefore, under the condition of a strong, in the sense of (12), nearest neighbour interaction in one direction, the classical partition function of a d + 1 D system (1) is given in the thermodynamic limit by the following expression

$$Z^{(d+1)}_{c\ell} = (\hbar^2\beta^2\Phi_0/m)^{N'/2}\exp(-\beta N_0\epsilon_0) , \tag{14}$$

where ϵ_0 is an energy of the ground state of an appropriate d D system (see Eqs. (9) and (10)).

Finally, we want to emphasize two points. Our result (14), which may be obtained within the Transfer Integral Method (TIM) should be justified and a particular justification might be given by using the above described procedure in an exactly soluble case, e.g., in the case of a system of harmonic oscillators (see also recent discussion by Bullough [3] and Henry and Oitmaa [4]). In a general case, the quantity (10) might be found by using the Bogolubov inequality

$$F \le F_0 + \langle H - H_0\rangle_0 ,$$

adopted for the limiting case, $\beta \to \infty$, then $F \to E_0$. There are at least two obvious variational methods of the type of independent sites and independent modes which might be used. In our next paper these two problems will be discussed in detail and the comparison of the results of the above presented treatment with these of methods of the type of mean field approximation will be given by an example of ϕ^4 model.

On the other hand, there is somewhat deeper problem: how far does this analogy between the properties of classical d + 1 D system and the properties of quantum dD system ($\beta \to \infty$) extend? Bishop and Krumhansl [5] in their discussion of 2D and 3D ϕ^4 model escaped of this question assuming a weak transverse coupling and thus reducing the model to 1D and 2D, respectively, Ising model in a transverse field at T = 0 [6]. In our opinion all intersting features such as correlation function or static susceptibility functions should be found for a quantum system in a region of low but finite temperatures, $T \neq 0$, and then the limit $T \to 0$ should be taken. In a forthcoming paper the correspondence between correlation functions and generalized isothermal susceptibilities for d + 1 D classical and d D quantum systems will be found. We shall show that the phase transition in d + 1 D system takes place when $E_1 \to E_0$ in an appropriate dD quantum system. This is expected,, $\{E_n\}$ denote eigenvalues of transfer integral operator, but not obvious result, as is seen when some approximating method is used (e.g., MFA used by Bishop and Krumhansl [5]).

Let us point out at the end one more or less trivial fact. The phase transition in a quantum d D system is driven by $\tilde{\hbar}$ (in our notation). Misunderstanding at this point caused that Guyer et al. [7] in their discussion of 2D one- and two-component ϕ^4 model have came to the conclusion that there is a phase transition at finite $T_c \neq 0$ in 1D ϕ^4 model. Evidently it is an artificial effect of their variational method.

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Радош А., Салейда В. E17-87-778

Статистическая сумма классической d+1-мерной системы структурного фазового перехода

Показано, что проблема вычисления статистической суммы классической d+1-мерной системы может быть сформулирована как задача Шредингера, соответствующая d-мерной системе. В термодинамическом пределе существенным d оказывается основное решение уравнения Шредингера.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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Radosz A., Salejda W. E17-87-778

On the Partition Function of d+1 Dimensional Kink-Bearing Systems

It is suggested that the problem of finding a partition function of d+1 dimensional kink-bearing system in the classical approximation may be formulated as an eigenvalue problem of an appropriate d dimensional quantum system.

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

Communication of the Joint Institute for Nuclear Research. Dubna 1987