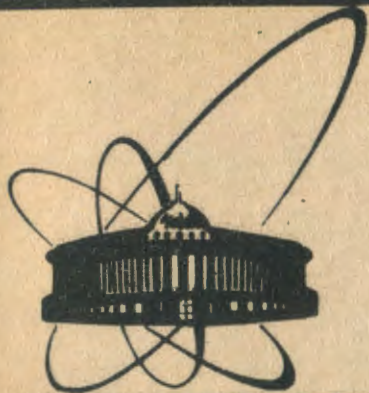


89-139



СООБЩЕНИЯ
ОБЪЕДИНЕННОГО
ИНСТИТУТА
ЯДЕРНЫХ
ИССЛЕДОВАНИЙ
ДУБНА

R 13

E17-89-139

A. Radosz

ON THE CLASS OF EXACTLY SOLUBLE MODELS
OF PHASE TRANSITIONS

1989

Some time ago, Sarbach and Schneider^{/1/} showed how the free energy of the class of models of phase transition with the Hamiltonian:

$$H = \sum_{\ell} \frac{P_{\ell}^2}{2M} + \frac{1}{4} \sum_{\ell_1} \phi_{\ell_1} (Q_{\ell} - Q_{\ell_1})^2 + NV \left(\frac{1}{N} \sum_{\ell} Q_{\ell}^2 \right), \quad (1)$$

where P_{ℓ} and Q_{ℓ} are canonically conjugated variables, N is the number of atoms and $V(x)$ is a well-defined potential, may be estimated exactly (see also^{/2/}).

These authors stated that the model (1) belongs to the class of universality of the spherical model, although there have existed some unsolved problems associated with the behaviour of susceptibility function. The temperature dependence of susceptibility has been widely discussed very recently^{/3,4/}.

In this note, starting from a definition of the partition function

$$Z = \text{Tr} \{ \exp(-\beta H_h) \}, \quad (2)$$

where a term of interaction with an external field h has been added

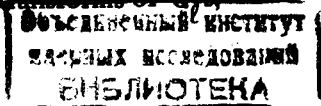
$$H_h = H - h \sum_{\ell} Q_{\ell}, \quad (2a)$$

the free energy for the model (1) is estimated within a part integral formalism without any limitation to the classical approximation. It seems that the result is exact in the thermodynamical limit but the arguments have rather a physical than mathematical character.

The partition function Z expressed as a path integral in imaginary time^{/5/} may be given by the following formulae:

$$Z = \int D[Q_q(\tau)] \exp\left(-\frac{1}{\hbar} S\right) = \lim_{L \rightarrow \infty} Z^{(L)}, \quad (3)$$

where Q_q 's are the Fourier transforms of Q_j 's,



$$S = \int_0^T dr \left\{ \sum_q \left(\frac{M}{2} \left[\frac{dQ_q^R}{dr} \right]^2 + \left(\frac{dQ_q^I}{dr} \right)^2 \right) + \frac{1}{2} (\phi_0 - \phi_q) Q_q Q_{-q} + \right. \\ \left. + NV \left(\frac{1}{N} \sum_q Q_{-q} Q_q \right) - \sqrt{N} \hbar Q_0 \right\} \quad (4)$$

$$Z^{(L)} = \int \prod_q dQ_q(L) \dots \int \prod_q dQ_q(1) \exp \left(-\frac{1}{\hbar} \sum_{n=1}^L \epsilon \times \right. \\ \times \left\{ \sum_q \frac{M}{2\epsilon^2} [Q_q(n) - Q_q(n-1)][Q_{-q}(n) - Q_{-q}(n-1)] - \sqrt{N} \hbar Q_0(n) + \right. \\ \left. + \frac{1}{2} (\phi_0 - \phi_q) Q_{-q}(n) Q_q(n) + NV \left(\frac{1}{N} \sum_q Q_{-q}(n) Q_q(n) \right) \right\} \Big|_{Q(L) \equiv Q(0)} \\ = \int_0^\infty dm_L \dots \int_0^\infty dm_1 \exp \left(-\frac{1}{\hbar} N \epsilon \sum_{i=1}^L V(m_i) \right) \int \prod_q dQ_q(L) \dots \int \prod_q dQ_q(1) \times \quad (5)$$

$$\prod_{i=1}^L \delta \left[m_i - \frac{1}{N} \sum_q Q_{-q}(i) Q_q(i) \right] \exp \left\{ -\frac{1}{\hbar} \sum_{i=1}^L \epsilon \left(\sum_q \left\{ \frac{1}{2} (\phi_0 - \phi_q) Q_{-q}(i) Q_q(i) + \right. \right. \right. \\ \left. \left. + \frac{M}{2\epsilon^2} [Q_{-q}(i) - Q_{-q}(i-1)][Q_q(i) - Q_q(i-1)] - \hbar \sqrt{N} Q_0(i) \right\} \right),$$

$$T \equiv \beta \hbar = L \cdot \epsilon. \quad (6)$$

Inserting a usual δ - representation

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{ikx},$$

into Eq.(5) one finds $Z^{(L)}$ in the form

$$Z^{(L)} = \int_0^\infty dm_L \dots \int_0^\infty dm_1 \exp[-\frac{1}{N} N \in \sum_{i=1}^L V(m_i)]$$

$$\frac{1}{2\pi} \int_{-\infty}^\infty dk_L \dots \frac{1}{2\pi} \int_{-\infty}^\infty dk_1 \exp(iN \sum_{n=1}^L m_n k_n) \times \quad (7)$$

$$\times (\prod_q Z_q^{(L)}) Z_h^{(L)},$$

$$\prod_q Z_q^{(L)} = \prod_q \int dQ_q(L) \dots \int \prod_q dQ_q(1) \exp(-\frac{1}{\hbar} \sum_q S_q^{(L)}) =$$

$$= \int \prod_q dQ_q(L) \dots \int \prod_q dQ_q(1) \exp\{-\frac{1}{\hbar} \sum_{n=1}^L \sum_q (\frac{M}{2\theta} [Q_{-q}(n) - Q_{-q}(n-1)] \times \quad (7a)$$

$$\times [Q_{+q}(n) - Q_{+q}(n-1)] + \frac{1}{2} \in M \omega_q^2(n) Q_{-q}(n) Q_{+q}(n)\},$$

$$Z_h = \exp[+\frac{1}{2\hbar} N \in \sum_{n=1}^L (\frac{\hbar^2}{\omega_o^2(n) M})], \quad (7b)$$

$$\omega_q^2(n) = \frac{1}{M} (\phi_o - \phi_q + 2ik_n \frac{\hbar}{c}).$$

As the calculation of $Z_q^{(L)}$ needs to take Gaussian integrals, the only problem, is to use a convenient notation. As a result one finds

$$Z_q^{(L)} = [A_q^{(L)} B_q^{(L)} - 2]^{-\frac{1}{2}}, \quad (8)$$

where

$$A_q^{(L)} = c_{(L)}(q) - [\frac{1}{c_1(q)} + \frac{1}{c_2(q) c_1(q)} + \dots + \frac{1}{c_{L-1}(q) c_{L-2}^2(q) \dots c_1^2(q)}] \quad (8a)$$

$$B_q^{(L)} = c_1(q) c_2(q) \dots c_L(q), \quad (8b)$$

$$c_1(q) = 2 + \omega_1^2(q) \in^2 \quad (8c)$$

$$c_n(q) = 2 + \omega_n^2(q) \in^2 - \frac{1}{c_{n-1}(q)}. \quad (8b)$$

By using in Eq.(7) Z_q in the form (8), one can see that the integral over all $k(n)$ takes the following form:

$$I = \int_{-\infty}^{\infty} dk_1 \dots \int_{-\infty}^{\infty} dk_L \exp[-Nf(\{k_n\})], \quad (9)$$

where

$$f(\{k_n\}) = -i \sum_{\ell} k_{\ell} m_{\ell} + \frac{1}{N} \sum_q \ln Z_q^{(L)} - \frac{\in}{2\hbar} \sum_{\ell=1}^L \frac{\hbar^2}{M\omega_{\ell}^2(0)}.$$

Let us assume that the estimation of integral (9) may be given by analogy with the saddle point method but extended to the $L -$ dimensional space. Then, the leading contribution to I is

$$I \simeq \exp[-Nf(\{k_n(0)\})]. \quad (10)$$

where $\{k_n(0)\}$, are functions of $m_n - s$ found from the condition

$$\frac{\partial f}{\partial k_n} \Big|_{\{k_i(0)\}} = 0. \quad (10a)$$

Therefore, the partition function $Z^{(L)}$ in this approximation to the leading term, (Eq. in (10)), is given by the following formulae:

$$Z^{(L)} \simeq \exp[-NF(\{m_i\})] \Big|_{m_i = m_i(0)}, \quad (11)$$

where

$$F(\{m_i(0)\}) = \frac{\in}{\hbar} \sum_{i=1}^L V(m_i(0)) + f(k_n(\{m_i(0)\})), \quad (11a)$$

and $\{m_i(0)\}$ correspond to the minimum of the function F

$$\left. \frac{\partial F}{\partial m_1} \right|_{m_n(0)} = 0 \Leftrightarrow ik_n(0) = \frac{\epsilon}{\hbar} V'(m_n(0)). \quad (11b)$$

Equation (11a) has the solution (see also Eq.(10a)).

$$ik_1(0) = ik_2(0) = \dots = ik_L(0) \equiv ik(0) = \frac{\epsilon}{\hbar} V'(m(0)). \quad (12a)$$

$$m_1(0) = m_2(0) = \dots = m_L(0) \equiv m(0) = \frac{1}{N} \sum_q \frac{B_q^{(L)}(0)}{A_q^{(L)}(0) B_q^L(0) - 2} +$$

$$+ \left[\frac{\hbar}{2V'(m(0))} \right]^2,$$

$$A_q^{(L)}(0) = A_q^{(L)}(c_n^\circ(q)), \quad B_q^{(L)}(0) = B_q^{(L)}(c_n^\circ(q)), \quad (12b)$$

$$c_n^\circ(q) \equiv c_n(q) \quad (k_1 = k_2 = \dots = k_n = k). \quad (12c)$$

In the limit, $\epsilon \rightarrow 0$ ($L \rightarrow \infty$), formulae (11) and (12a-c) allow one to obtain a free energy function \mathcal{F} in the form

$$\mathcal{F} = - \frac{k_B T}{N} \ln Z =$$

$$= - \frac{k_B T}{N} \sum_q \ln \left[2 \operatorname{sh} \left(\frac{\hbar \omega_q}{2k_B T} \right) \right] + [V(m(0)) - mV'(m(0))] - \frac{1}{2} \frac{\hbar^2}{2V'(m(0))}, \quad (13)$$

where

$$m(0) = \frac{1}{N} \sum_q \frac{\hbar}{2\omega(q)} \operatorname{cth} \left(\frac{\hbar \omega(q)}{2k_B T} \right) + \left[\frac{\hbar}{2V'(m(0))} \right]^2 \quad (13a)$$

$$\omega^2(q) = \frac{1}{M} [\phi_0 - \phi_q + 2V'(m(0))].$$

This result Eq.(13), is expected to be exact in the thermodynamical limit. We cannot prove it, as we are not able to extend the saddle point method to the L-dimensional space ($L \rightarrow \infty$) and also to show that the solution (12b) corresponds to the minimum of the function F. However, there are other arguments justifying our statement: Firstly, in the classical approximation, $k_B T \gg \hbar \omega(q)$ the well-known result

$$\mathfrak{F} = \frac{k_B T}{N} \sum_q \ln \left(\frac{\hbar \omega(q)}{k_B T} \right) + [V(m(0)) - V'(m(0)) m(0)] - \frac{1}{2} \frac{\hbar^2}{2V'(m(0))}, \quad (14)$$

$$m(0) = \frac{k_B T}{N} \sum_q \omega^{-2}(q) + \left[\frac{\hbar}{2V'(m(0))} \right]^2, \quad (14a)$$

$$\omega^2(q) = \frac{1}{M} [\phi_0 - \phi_q + 2V'(m(0))], \quad (14b)$$

is reproduced (see ^{1,2/} and ^{4/}). Secondly, in the special case

$$V(x) = -\frac{A}{2} x + \frac{B}{4} x^2, \quad (15)$$

the exact solution was found within approximating Hamiltonian method by Plakida and Tonchev ^{6/}. Their result is the same as our result (13).

Let us emphasize at the end that because of the form of this paper some mathematical details, especially corresponding to the derivation of formulae (8) and (12a), have been omitted. Detailing discussion and somewhat deeper mathematical arguments justifying the result (13) will be given elsewhere.

The work was carried out under contract CPBP 01.02.

REFERENCES

1. Sarbach S., Schneider T. - *Phys. Rev. B*, 1977, 17, p.347.
2. Van Hemmen J.L., Zagrebnev V.A. - *Preprint 425, Universitat Heidelberg*, 1987.

3. Radosz A. – *Phys. Lett. A*, 1988, 127, p.319.
4. Radosz A. – 1988, unpublished.
5. Feynman R.P., Hibbs A.R. – *Quantum Mechanics and Path Integrals*, McGraw Hill, N.Y., 1965.
6. Plakide N.M., Tonchev N.S. – *Theor. Mat. Fiz.*, 1985, 68, p.270; *Physica*, 1986, 136A, p.176.

Received by Publishing Department
on March 2, 1989.