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APPLICATION OF A FUNCTIONAL ANALOG OF THE VARIATIONAL PRINCIPLE OF N.N.BOGOLUBOV TO THE φ^4 MODEL

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Применение функционального аналога вариационного метода Боголюбова к модели ϕ^4

Исходя из развитого в предыдущих работах функционального аналога вариационного метода Боголюбова изучается модель ϕ^4 в парамагнитной области. В качестве вариационного функционала употребляется биквадратный функционал с расцепляющимися модами. Решаются уравнения для вариационных параметров и получаются выражения для свободной энергии и парной корреляционной функции, откуда получаются поправка к критической температуре /относительно теорий среднего поля/ и значения критических индексов. Результаты обобщаются на случаи модели с членами ϕ^6, ϕ^8 и т.д.

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Application of a Functional Analog of the Variational Principle of N.N.Bogolubov to the ϕ^4 Model

A functional analog of the variational principle of N.N.Bogolubov is applied to the ϕ^4-model using a biquadratical functional with non-iteracting modes. A correction to the critical temperature and the critical indices are obtained. The results are generalized to other models.

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

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1. Introduction

In paper[1] it was obtained that for a large class of systems the free energy can be written as

$$F = F_0 + \tilde{F}, \qquad 1\text{-}1$$

where F_0 is the free energy in the mean field theory and $\tilde{F}$ is the contribution of fluctuations for which was obtained the functional integral representation

$$e^{-\beta\tilde{F}} = \int \mathcal{D}\xi_x \, e^{-\varphi[\xi_x]} \, . \qquad 1\text{-}2$$

When we are interested in critical behaviour of the system, fluctuations are large and perturbation theory is not useful in evaluating 1-2. For this case it has been proposed[2] a variational method which represents a functional analog of the variational principle of N.N.Bogoliubov and obtained the inequality

$$\tilde{F} \leq \frac{1}{\beta}\langle \varphi_\eta - \psi \rangle_\psi - \frac{1}{\beta}\ln \int \mathcal{D}\eta_y \, J(\eta_y)\, e^{-\psi[\eta_y]}, \qquad 1\text{-}3$$

where ψ is a functional of the new field η_y for which we suppose that integrals appearing in 1-3 can be calculated and which depends on some parameters. The new field η_y is related to ξ_x by the functional transformation

$$\eta_y = U_t(\xi_x, y) \qquad 1\text{-}4$$

whose Jacobian $J(\eta_y)$ is supposed to be positive. The condition of minimum of the right-hand side of(1-3) leads to equations determining the parameters contained in ψ and t whose general form is

$$\langle\langle \delta\psi ; (\phi-\psi)\rangle\rangle_\psi = 0 \qquad 1\text{-}5$$

$$\langle\langle (\phi-\psi) ; \frac{\partial \ln J}{\partial t}\rangle\rangle_\psi = \langle \frac{\partial}{\partial t}(\ln J - \phi)\rangle_\psi \ , \qquad 1\text{-}6$$

where $\langle\langle A;B\rangle\rangle = \langle A\rangle\langle B\rangle - \langle AB\rangle$

In the present paper we will consider a particular type of functional ψ and transformation of field η and will apply the method to the ϕ^4 model.

2. Biquadratical Trial Functional with Non-Interacting Modes

Let us suppose that the field ξ depends only on d-dimensional space coordinate x and define the new field

$$\eta(q) = \frac{1}{L^{d/2}}\int \xi(x)\, e^{-iqx}\, dx \qquad 2\text{-}1$$

and the functional

$$\psi[\eta] = \frac{1}{2}\sum_q r(q)\,|\eta(q)|^2 + A(q)\,|\eta(q)|^4 \ , \qquad 2\text{-}2$$

where $r(q)$ is fixed and $A(q)$ is the varational parameter. The functional 2-2 includes interaction between fluctuation in such a way that different modes do not interact one with the other. In this case $J(\eta)$ is a constant. Differentiating 1-3 with respect to $A(q)$ we obtain the equation

$$\langle\langle \varphi_\eta ; |\eta(q)|^4\rangle\rangle_\psi = \langle\langle \psi ; |\eta(q)|^4\rangle\rangle_\psi \ . \qquad 2\text{-}3$$

The right-hand side of 2-3 can be written explicitly

$$\langle\langle \psi ; |\eta(q)|^4\rangle\rangle_\psi = \frac{1}{2}\sum_{q_1} r(q_1)\langle\langle |\eta(q_1)|^2 ; |\eta(q)|^4\rangle\rangle_\psi + A(q_1)\langle\langle |\eta(q_1)|^4 ; |\eta(q)|^4\rangle\rangle_\psi \qquad 2\text{-}4$$

All means and correlators can be obtained by differentiating

$$I = \int \prod_q d\eta(q)\, \exp\left\{-\frac{1}{2}\sum_q r(q)\,|\eta(q)|^2 + A(q)\,|\eta(q)|^4\right\} \qquad 2\text{-}5$$

in particular:

$$\langle |\eta(q)|^2\rangle_\psi = -\frac{\delta \ln I}{\delta r(q)} \qquad 2\text{-}6a$$

$$\langle\langle |\eta(q)|^2 ; |\eta(q')|^2 \rangle\rangle_\psi = \frac{\delta^2 \ln I}{\delta r(q)\, \delta r(q')} \quad , \qquad \text{2-6b}$$

$$\langle\langle |\eta(q)|^2 ; |\eta(q')|^4 \rangle\rangle_\psi = \frac{\delta^2 \ln I}{\delta r(q)\, \delta A(q')} \quad , \qquad \text{2-6c}$$

$$\langle\langle |\eta(q)|^4 ; |\eta(q')|^4 \rangle\rangle_\psi = \frac{\delta^2 \ln I}{\delta A(q)\, \delta A(q')} \quad , \qquad \text{2-6d}$$

where we have supposed that $r(q) = r(-q)$ and $A(q) = A(-q)$

Now, 2-5 is easily integrable in terms of error function to obtain

$$\ln I = \frac{1}{2} \sum_q \ln \left\{ (-\pi^3)^{1/2} \frac{e^{s_q^2}}{A^{1/2}(q)} \left[1 - \mathrm{erf}(s_q) \right] \right\} \qquad \text{2-7}$$

with $s_q = \dfrac{r(q)}{2\, A^{1/2}(q)}$. Making use of equations 2-6 we obtain

$$\langle |\eta(q)|^2 \rangle_\psi = \varphi_0(s_q)\, A^{-1/2}(q) \qquad \text{2-8a}$$

$$\langle\langle |\eta(q)|^2 ; |\eta(q')|^2 \rangle\rangle_\psi = \varphi_1(s_q)\, A^{-1}(q)\, \Delta(q,q') \qquad \text{2-8b}$$

$$\langle\langle |\eta(q)|^2 ; |\eta(q')|^4 \rangle\rangle_\psi = \varphi_2(s_q)\, A^{-3/2}(q)\, \Delta(q,q') \qquad \text{2-8c}$$

$$\langle\langle |\eta(q)|^4 ; |\eta(q')|^4 \rangle\rangle_\psi = \varphi_3(s_q)\, A^{-2}(q)\, \Delta(q,q') \, , \qquad \text{2-8d}$$

where

$$\Delta(q,q') = \Delta(q+q') + \Delta(q-q') \qquad \text{2-9}$$

$$\mathrm{erf}(s) = \frac{2}{\sqrt{\pi}} \int_0^s dt\, e^{-t^2} \quad ; \quad z(s) = \frac{1}{\sqrt{\pi}} \frac{e^{-s^2}}{1-\mathrm{erf}(s)} \qquad \text{2-10}$$

$$\varphi_0(s) = z(s) - s \qquad \text{2-11a}$$

$$\varphi_1(s) = \frac{1}{2} + s\, z(s) - z^2(s) \qquad \text{2-12a}$$

$$\varphi_2(s) = -s + \frac{1}{2} z(s) - s^2 z(s) + s\, z^2(s) \qquad \text{2-13a}$$

$$\varphi_3(s) = \frac{1}{2} + 2s^2 - \frac{3s}{2} z(s) + s^3 z(s) - s^2 z^2(s) \quad . \qquad \text{2-14a}$$

In forthcoming applications we will deal also with expressions of the type

$$R_n^m(q) = \frac{1}{L^{d(n-1)}} \sum_{q_1 \cdots q_{2n}} \Delta(q_1 + \cdots + q_{2n}) \langle\langle \eta(q_1) \cdots \eta(q_{2n}) ; |\eta(q)|^{2m} \rangle\rangle_\psi \qquad 2\text{-}15$$

$$S_n = \frac{1}{(L^d)^n} \sum_{q_1 \cdots q_{2n}} \Delta(q_1 + \cdots + q_{2n}) \langle \eta(q_1) \cdots \eta(q_{2n}) \rangle_\psi \qquad 2\text{-}16$$

for which in the limit $L \to \infty$ the following results are obtained

$$R_n^m(q) = 2n(2n-1)!! \langle\langle |\eta(q)|^2 ; |\eta(q)|^{2m} \rangle\rangle_\psi \left[\int \frac{d^d p}{(2\pi)^d} \langle |\eta(p)|^2 \rangle_\psi \right]^{n-1} \qquad 2\text{-}17$$

$$S_n = (2n-1)!! \left[\int \frac{d^d p}{(2\pi)^d} \langle |\eta(p)|^2 \rangle_\psi \right]^n \qquad 2\text{-}18$$

3. Application to the φ^4 -Model

We now consider the particular case[3]

$$\Phi(\xi) = \frac{1}{2} \int dx \left\{ \tau \xi^2(x) + (\nabla \xi)^2 + 2u \xi^4(x) \right\} \qquad 3\text{-}1$$

and write this functional in terms of $\eta(q)$

$$\varphi_\eta = \frac{1}{2} \sum_q (\tau + q^2) |\eta(q)|^2 + \frac{u}{L^d} \sum_{q_1 \cdots q_4} \Delta(q_1 + \cdots + q_4) \eta(q_1) \cdots \eta(q_4) \;. \qquad 3\text{-}2$$

Here $\tau = a \frac{\theta - \theta_c^0}{\theta_c^0}$ where θ_c^0 is the critical temperature in the mean field approximation and $a, u > 0$. Substituting 3-2 in 2-3, considering $r(q) = \tau + q^2$ and using the results of previous section we obtain for $A(q)$ the equation

$$A^{1/2}(q) = 12u \frac{\varphi_2(s_q)}{\varphi_3(s_q)} \int \frac{d^d p}{(2\pi)^d} \varphi_0(s_p) A^{-1/2}(p) \;. \qquad 3\text{-}3$$

This equation can not be solved in the general case to obtain $A(q, \theta)$ but in the neighbourhood of the critical point all necessary information can be obtained from it.

The pair correlation function $\Gamma(q, \theta)$ which in this approximation is

$$\Gamma(q, \theta) = \langle |\eta(q)|^2 \rangle_\psi \qquad 3\text{-}4$$

must satisfy in the critical point the equation

$$\frac{1}{\Gamma(0,\theta_c)} = 0 \qquad \text{3-5}$$

this implies that when $\theta \Rightarrow \theta_c$ and $q \to 0$, $r(q,\theta_c)<0$, $A(q,\theta_c) \to 0$ and $S_q(\theta_c) \to -\infty$. Then replacing the functions φ_2 and φ_3 by their asymptotics when $S \to -\infty$

$$\varphi_2(S) \approx -S$$
$$\varphi_3(S) \approx \frac{1}{2} + 2S^2 \qquad \text{3-6}$$

we obtain for $\theta = \theta_c$ and $q = 0$

$$r(0,\theta_c) = -\frac{12u}{(2\pi)^d}\int d^d q\, \Gamma(q,\theta_c) \qquad \text{3-7}$$

meaning that

$$\frac{\theta_c}{\theta_c^0} = 1 - \frac{12u}{a(2\pi)^d}\int d^d q\ \Gamma(q,\theta_c) \qquad \text{3-8}$$

for $\theta = \theta_c$ and small q we have

$$\Gamma(q,\theta_c) = \varphi_0(S_q)\ \frac{2S_q(\theta_c)}{r(q,\theta_c)}$$

$$\Gamma(q,\theta_c) \approx -\ \frac{2S_q^2(\theta_c)}{r(q,\theta_c)} \qquad \text{3-9}$$

and from 3-3, 3-6, 3-7

$$2S_q^2(\theta_c) = \frac{r(q,\theta_c)}{2\left[r(q,\theta_c) - r(0,\theta_c)\right]}$$

then

$$\Gamma(q,\theta_c) \approx \frac{1}{2q^2} \qquad \text{3-10}$$

This means that the critical index $\eta = 0$. Using eq.3-10 in 3-8 and introducing a cut off wave vector q_0 we obtain for $d = 3$

$$\frac{\theta_c}{\theta_c^0} = 1 - \frac{3uq_0}{\pi a}\ . \qquad \text{3-11}$$

Consider now $\theta \approx \theta_c$ and small q . From 3-3 and 3-6

$$\Gamma(q,\theta) = \frac{1}{2}\ \frac{1}{q^2 + \lambda^{-2}}\ , \qquad \text{3-12}$$

where the correlation length λ is given by

$$\frac{1}{\lambda^2} = r(0,\theta) + \frac{12u}{(2\pi)^d}\int d^d q\, \Gamma(q,\theta) \qquad 3\text{-}13$$

Using 3-7, 3-10 and 3-12 we obtain

$$\frac{1}{\lambda^2} + b(d)\,\lambda^{2-d} = a\,\frac{\theta-\theta_c}{\theta_c^\circ} \qquad 3\text{-}14$$

which implies that $\lambda \sim (\theta-\theta_c)^{\frac{1}{2-d}}$ meaning that the critical index ν is

$$\nu = \frac{1}{d-2} \qquad 3\text{-}15$$

when d =4 we have again the mean field value $\nu = \frac{1}{2}$ and for d =3, ν =1. Formulae 3-14, 3-15 are not valid for d =2. The susceptibility $\chi(\theta)$ is given by

$$\chi(\theta) = \frac{\lambda^2}{2\theta} \qquad 3\text{-}16$$

so that the corresponding index $\gamma = \frac{2}{d-2}$

The specific heat can be obtained using

$$C_\varphi = -\frac{\theta}{L^d}\,\frac{\partial^2 F(\psi)}{\partial\theta^2} \qquad (3\text{-}17$$

$$F(\psi) = \theta\,\langle \varphi_\eta - \psi \rangle_\psi - \theta \ln \int \mathcal{D}\eta\, e^{-\psi}, \qquad 3\text{-}18$$

resulting that the critical index α is equal to zero. Now from $\delta = (d+2-\eta)/(d-2+\eta)$ it follows that $\delta = (d+2)/(d-2)$ and from $\beta\delta = \beta + \gamma$ that β =1/2.

4. Generalization and Concluding Remarks

The results of previous section are easilly generalizable to more general functionals as, for example,

$$\Phi(\xi) = \frac{1}{2}\int d^d x \left\{ \tau\xi^2(x) + (\nabla\xi)^2 + \sum_{n=1}^{\infty} u_n\, \xi^{2n+2}(x) \right\} \qquad 4\text{-}1$$

using the formulae of section 2 we obtain for $A(q)$

$$\overset{1/2}{A}(q)=\frac{\varphi_2(S_q)}{\varphi_3(S_q)}\sum_{n=1}^{\infty}n(2n-1)!!\,u_n\left[\int\frac{d^dp}{(2\pi)^d}\varphi_0(S_p)\overset{-1/2}{A}(p)\right]^n \tag{4.2}$$

and for the critical temperature

$$\frac{\Theta_c}{\Theta_c^o}=1-\sum_{n=1}^{\infty}n(2n-1)!!\,u_n\left[\frac{1}{(2\pi)^d}\int\frac{d^dp}{2p^2}\right]^n. \qquad 4\text{-}3$$

The critical indices will be the same as in previous section

$$\alpha=0 \qquad \gamma=\frac{2}{d-2} \qquad \eta=0$$

$$\beta=\frac{1}{2} \qquad \delta=\frac{d+2}{d-2} \qquad \nu=\frac{1}{d-2} \qquad 4\text{-}4$$

They are characteristic of the trial functional 2-2 used here and do not depend on Φ because all are determined from the pair correlation function which in this approach is simply $\langle|\eta(q)|^2\rangle_\psi$ depending on Φ only through parameters as α, Θ_c^o, u_n which are irrelevant in critical behavour.

Note that the set of indices 4-4 coincides for the special dimension $d=4$ with those of the Gaussian approximation. If we use 2-2 as zero order approximation to obtain the renormalization group equations, the resulting ϵ -expansion for the critical indices will be the same as in Wilson's approach because for $d=4$ 2-2 and the Gaussian functional are equivalent.

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