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# GENERATING FUNCTIONAL AND FUNCTIONAL ANALOG OF THE VARIATIONAL PRINCIPLE OF N.N.BOGOLUBOV

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Производящий функционал и функциональный аналог вариационного метода Боголюбова

Вводится производящий функционал, с помощью которого получаются функциональные представления для статистической суммы и других величин широкого класса моделей статистической механики. Перечисляются те приближенные методы, которые обычно используются при вычислении континуальных интегралов полученного типа, и предлагается новый вариационный метод, являющийся функциональным аналогом вариационного метода Боголюбова. Получаются общие уравнения для вариационных параметров. Рассматриваются некоторые возможные варианты преобразования полей, а также приводится несколько примеров вариационного функционала. Метод иллюстрируется на некоторых нетривиальных моделях.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

**Препринт Объединенного института ядерных исследований. Дубна 1979**

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Fedyanin V.K., Mochinsky B.V., Rodriguez C. **E17 - 12850**

Generating Functional and Functional Analog of the Varioational Principle of N.N.Bogolubov

A generating functional is introduced and functional integral representations for the thermodynamical quantities and correlation functions of a large class of systems are obtained. A functional analog of the variational principle of N.N.Bogolubov is developed and applied to some non-trivial models of statistical mechanics.

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

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Starting from a generating functional introduced in this paper, a functional analog of the variational principle of N.N.Bogolubov for path integral applications in statistical mechanics is developed. The method is illustrated by applying it to some non-trivial models.

1. Let's consider a system whose Hamiltonian $\hat{H}$ can be written as $\hat{H}=\hat{H}_0+\hat{H}_i$, where $\hat{H}_0$ is a one-particle Hamiltonian and $\hat{H}_i$ is an interaction of the type:

$$\hat{H}_i = -\frac{1}{2}\int d\bar{r}\, d\bar{r}' \sum_{jj'} J_{jj'}(\bar{r}-\bar{r}')\hat{\mathcal{L}}_{j\bar{r}}\hat{\mathcal{L}}^{+}_{j'\bar{r}'}, \tag{1}$$

where $\hat{\mathcal{L}}_{j\bar{r}}$, $\hat{\mathcal{L}}^{+}_{j\bar{r}}$ are linearly independent operators, and $J_{jj'}(\bar{r}-\bar{r}')$ is a pair interaction potential. The specific form of $\hat{\mathcal{L}}_{j\bar{r}}$, $\hat{\mathcal{L}}^{+}_{j\bar{r}}$ is determined by the system under study.

For example, for magnetic systems $\hat{\mathcal{L}}_{j\bar{r}}$ are spin density operators or, in general, Racah operators; for a system of interacting bosons or fermions they are particle density operators (the index j denotes the kind of particle and the spin), in the case of a superconductor $\hat{\mathcal{L}}_{j\bar{r}}$, $\hat{\mathcal{L}}^{+}_{j\bar{r}}$ are the annihilation and creation operators of Cooper's pairs. In order to obtain a functional integral representation for the partition function and the correlators of the system, we introduce the generating functional

$$Z(\ell, \ell^*) = \mathrm{Sp}[e^{-\beta\hat{H}_0}\, T\exp\{-g\int_0^\beta H_i(\tau)\,d\tau - \sum_x \ell(x)\hat{\mathcal{L}}_x + \ell^*(x)\hat{\mathcal{L}}^{+}_x\}] \tag{2}$$
$$x = j,\bar{r},\tau;\ \bar{r}\in V;\quad 0\le\tau\le\beta,$$

where all operators are in the interaction picture

$$\hat{A}(\tau) = \exp(\tau\hat{H}_0)\hat{A}\exp(-\tau\hat{H}_0) \tag{3}$$

and the trace is performed in the space of $\mathcal{L}_{j\bar{r}}$. We will consider that $\mathcal{L}_{j\bar{r}}$ are Bose operators

$$[\mathcal{L}_{j\bar{r}}, \mathcal{L}_{j'\bar{r}'}]_- = [\hat{\mathcal{L}}^{+}_{j\bar{r}}, \mathcal{L}^{+}_{j'\bar{r}'}]_- = 0$$

and the functions $\ell(x)$ belong to the Hilbert space L of all complex functions satisfying the conditions

$$\ell_j(\bar{r}, \tau) = \ell_j(\bar{r}, \tau+\beta),$$

$$\sum_x |\ell(x)|^2 \equiv \int_V d\bar{r} \sum_j \int_0^\beta d\tau \, |\ell_j(\bar{r}, \tau)|^2 < \infty.$$

The partition function can be easily obtained from (2) in the way

$$Z = Z(\ell = 0, \ \ell^* = 0)|_{g=1} = \mathrm{Sp}\{e^{-\beta \hat{H}_0} \, \mathrm{T}\exp[-\int_0^\beta \hat{H}_i(\tau) d\tau]\}. \tag{4}$$

Expressions for all the averages, correlations and Matsubara's Green function can be derived taking the variational derivative of (2) with respect to $\ell(x)$ and $\ell^*(x)$ and then putting $\ell(x) = \ell^*(x) = 0$. For example,

$$\langle \mathcal{L}_{jr} \rangle = -\frac{\delta \ln Z(\ell, \ell^*)}{\delta \ell(x)}\Big|_{\ell, \ell^* = 0} \ ; \ \langle \mathcal{L}^+_{jr} \rangle = -\frac{\delta \ln Z(\ell, \ell^*)}{\delta \ell^*(x)}\Big|_{\ell, \ell^* = 0} . \tag{5}$$

From (2) it follows that $Z(\ell, \ell^*)$ satisfies the functional differential equation

$$\frac{\partial Z}{\partial g} = \frac{1}{2} \int_0^\beta d\tau \iint_V d\bar{r} d\bar{r}' \sum_{j,j'} J_{jj'}(\bar{r} - \bar{r}') \frac{\delta^2 Z}{\delta \ell(x) \delta \ell^*(x')} \tag{6}$$

with the initial condition

$$Z(\ell, \ell^*)|_{g=0} = Z_0(\ell, \ell^*) \equiv \mathrm{Sp}\{e^{-\beta \hat{H}_0} \mathrm{T}\exp[-\sum_x \ell(x) \hat{\mathcal{L}}_x + \ell^*(x) \hat{\mathcal{L}}^+_x]\}.$$

The formal solution of (6) is given by the functional integral

$$Z(\ell, \ell^*) = \int \mathfrak{D}m \mathfrak{D}m^* \exp[-\Phi_0(m, m^*)] Z_0(\ell + m, \ \ell^* + m^*),$$

$$\Phi_0(m, m^*) = \frac{1}{2} \int_0^\beta d\tau \iint_V d\bar{r} d\bar{r}' \sum_{jj'} m_j(\bar{r}, \tau) J^{-1}_{jj'}(\bar{r} - \bar{r}') m^*_{j'}(\bar{r}, \tau), \tag{7}$$

where the normalization is taken in such a way that for $Z_0 = 1$, $Z = 1$. The functional $Z_0$ has the meaning of the partition function of a system with Hamiltonian $H_0$ under the influence of external random fields $\ell(x), \ell^*(x)$. The partition function of the system with Hamiltonian $H = H_0 + H_i$ using (4) and (7) can be written as:

$$Z = \int \mathfrak{D}m \mathfrak{D}m^* \exp[-\Phi_0(m, m^*)] Z_0(m, m^*). \tag{8}$$

So that the selection of the interaction in the form (1) leads to a representation for the partition function Z as a functional integral of the functional $Z_0(\ell,\ell^*)$ over the space with a Gaussian measure.

2. The representation (8) allows us to introduce the "free energy functional" of the system:

$$\Phi(m,m^*) = \Phi_0(m,m^*) + \Phi_1(m,m^*)$$
$$\Phi_1(m,m^*) = -\ln \mathrm{Sp}\{e^{-\beta \hat{H}_0}\, \mathrm{T}\exp[-\sum_x m(x)\hat{\mathfrak{L}}_x + m^*(x)\hat{\mathfrak{L}}_x^+]\}. \tag{9}$$

Then the partition function and the free energy of the system are given by

$$Z = \int \mathfrak{D}m\mathfrak{D}m^*\, e^{-\Phi(m,m^*)},$$
$$F = -\theta \ln \int \mathfrak{D}m\mathfrak{D}m^*\, e^{-\Phi(m,m^*)}. \tag{10}$$

From (9) and the usual definition of $<\hat{A}>$ we can obtain expressions for the averages and correlators. For example, for $<\hat{\mathfrak{L}}_x>$ we have:

$$<\mathfrak{L}_{j\bar{r}}(\tau)> \equiv \frac{\mathrm{Sp}\,\mathfrak{L}_{j\bar{r}}e^{-\beta\hat{H}}}{\mathrm{Sp}\, e^{-\beta\hat{H}}} = -\frac{1}{2}\int d\bar{r}'\sum_{j'} J^{-1}_{jj'}(\bar{r}-\bar{r}')\frac{\int \ell_{j'\bar{r}'}(\tau)e^{-\Phi}\mathfrak{D}\ell\mathfrak{D}\ell^*}{\int e^{-\Phi}\mathfrak{D}\ell\mathfrak{D}\ell^*}. \tag{11}$$

Note that the trace in the definition of the functional $Z_0$ can be calculated only for a relatively small class of models. For example, it can be calculated for Ising's model, where:

$$\hat{H}_0 = -h\sum_{\bar{r}} S^z_{\bar{r}};\quad \hat{H}_i = -\frac{1}{2}\sum_{\bar{r}\bar{r}'} J(\bar{r}-\bar{r}')S^z_{\bar{r}}S^z_{\bar{r}'},$$

(here $S^z_{\bar{r}}$ is the z component of spin S at site $\bar{r}$):

$$\mathfrak{L}_{j\bar{r}} = S^z_{\bar{r}} \qquad \ell_j(\bar{r},\tau) = \ell(\bar{r});$$

we have

$$\Phi_1 = -\sum_{\bar{r}} B(\ell_{\bar{r}});\quad B(x) = \ln\sum_{m=-s}^{m=s} e^{\beta(h+x)m}.$$

Even in the cases for which the trace can be calculated to obtain an explicit expression for $\Phi_1$, the resulting functional integrals are not exactly calculable. Let's characterize some of the approximations usually employed in calculating functional integrals of this kind.

A. Perturbation Theory

Developing $\exp.(-\Phi_1)$ in a functional series, we have

$$e^{-\Phi_1} = \mathrm{Sp}\, e^{-\beta \hat{H}_o}[1 + \sum_x (\ell_x \langle \hat{\mathfrak{L}}_x \rangle_0 + \ell^*_x \langle \hat{\mathfrak{L}}^+_x \rangle_0) + \dots],$$

where

$$\langle \dots \rangle_0 = \frac{\mathrm{Sp}(e^{-\beta \hat{H}_o} \dots)}{\mathrm{Sp}\, e^{-\beta \hat{H}_o}}.$$

We suppose that all averages appearing in the above series are calculable. Then, we obtain a perturbation series for the free energy $F$ whose terms are proportional to functional integrals of the type:

$$\int \mathfrak{D}\ell \mathfrak{D}\ell^* e^{-\Phi_o(\ell,\ell^*)} \ell^*_{x_1}, \dots, \ell^*_{x_s} \ell_{y_1}, \dots, \ell_{y_s}$$

which are easily calculable using Wick's theorem (see refs. /1-4/ ). Analogous expressions can be obtained for the correlation functions.

B. Method of steepest descent

This method is a generalization of the method of steepest descent for multiple integrals to functional integrals (see ref. /5/ ). Let's consider the set of functions $\{\bar{\ell}_x, \bar{\ell}^*_x\}$ for which the functional $\Phi(\ell_x, \ell^*_x)$ has a minimum. They satisfy the system of equations

$$\frac{\delta\Phi}{\delta\ell_x} = 0 \qquad \frac{\delta\Phi}{\delta\ell^*_x} = 0,$$

or, more explicitly:

$$\frac{1}{2}\int_V d\bar{r}' \sum_{j'} J^{-1}_{jj'}(\bar{r}-\bar{r}')\, \bar{\ell}^*_{j'}(\bar{r}',\tau) = \frac{\mathrm{Sp}[e^{-\beta\hat{H}_o} T\exp\{-\sum_x \bar{\ell}_x \hat{\mathfrak{L}}_x + \bar{\ell}^*_x \hat{\mathfrak{L}}^+_x\} \hat{\mathfrak{L}}_{j\bar{r}}(\tau)]}{\mathrm{Sp}[e^{-\beta\hat{H}_o} T\exp\{-\sum_x \bar{\ell}_x \hat{\mathfrak{L}}_x + \bar{\ell}^*_x \hat{\mathfrak{L}}^+_x\}]},$$

$$\frac{1}{2}\int_V d\bar{r}' \sum_{j'} J^{-1}_{jj'}(\bar{r}-\bar{r}')\, \bar{\ell}_{j'}(\bar{r}',\tau) = \frac{\mathrm{Sp}[e^{-\beta\hat{H}_o} T\exp\{-\sum_x \bar{\ell}_x \hat{\mathfrak{L}}_x + \bar{\ell}^*_x \hat{\mathfrak{L}}^+_x\} \hat{\mathfrak{L}}^+_{j\bar{r}}(\tau)]}{\mathrm{Sp}[e^{-\beta\hat{H}_o} T\exp\{-\sum_x \bar{\ell}_x \hat{\mathfrak{L}}_x + \bar{\ell}^*_x \hat{\mathfrak{L}}^+_x\}]}.$$

We will suppose that $\ell_x, \bar{\ell}^*_x$ do not depend on $\tau$

$$\ell_j(\bar{r},\tau) = \ell_j(\bar{r})$$

then equations (11) determining $\ell, \ell^*$ become

$$\langle \mathfrak{L}_{j\bar{r}} \rangle_{\bar{H}} = \frac{1}{2}\int_V d\bar{r}' \sum_{j'} J^{-1}_{jj'}(\bar{r}-\bar{r}')\ell^*_j(\bar{r},\tau),$$

$$<\hat{\mathfrak{L}}^{+}_{j\bar{r}}> \quad = \frac{1}{2} \int_V d\bar{r}' \sum_{j'} J^{-1}_{jj'}(\bar{r}-\bar{r}')\bar{\ell}_j(\bar{r}')$$

Here $<...>_{\bar{H}}$ is the statistical average with an effective Hamiltonian $\bar{H}$:

$$\bar{H} = \hat{H}_0 + \int_V d\bar{r} \sum_j [\bar{\ell}_j(\bar{r})\hat{\mathfrak{L}}_{j\bar{r}} + \ell^*_j(\bar{r})\hat{\mathfrak{L}}^{+}_{j\bar{r}}(r)].$$

If we change in (9) $\Phi(\ell,\ell^*)$ by its minimum value $\Phi(\bar{\ell},\bar{\ell}^*)$ we obtain the expression for the free energy in the first approximation of this method

$$F = \theta\Phi(\ell,\ell^*); \; \Phi(\ell,\ell^*) = \frac{\beta}{2} \iint_V d\bar{r}d\bar{r}' \sum_{jj'} J^{-1}_{jj'}(\bar{r}-\bar{r}')\bar{\ell}_j(\bar{r})\bar{\ell}^*_j(\bar{r}') - \ln \operatorname{Sp} e^{-\beta\bar{H}}.$$

This approximation corresponds to a mean field (molecular field) approximation $\bar{\ell},\bar{\ell}^*$ for the operators $\hat{\mathfrak{L}},\hat{\mathfrak{L}}^+$. Note, that for some model systems this approximation is exact in the thermodynamical limit (see refs. /6,7/ ).

The next term in this method takes into account Gaussian fluctuations in the system. The corresponding contribution to the free energy is given by the Gaussian functional integral

$$F_G = -\theta \ln \int \mathfrak{D}\xi\, \mathfrak{D}\xi^* \exp\{-\frac{1}{2}\sum_{xx'} K(x,x')\xi_x\xi^*_{x'}\},$$

$$K(x,x') = \frac{\delta^2\Phi(\ell_x,\ell^*_x)}{\delta\ell_x\delta\ell^*_x}\Big|_{\substack{\ell_x=\bar{\ell}_x \\ \ell_x=\bar{\ell}_x}} \; ; \ell_x = \bar{\ell}_x + \xi_x; \; \ell^*_x = \bar{\ell}^*_x + \xi^*_x,$$

which in most cases is easily calculable. All subsequent terms are also expressed in terms of Gaussian functional integrals and give the contribution to free energy from the interaction between fluctuations. Now we pass to formulate an approximation method for the calculation of functional integrals which we have called the functional analog of the variational method of Bogolubov.

3. Let $\psi[\eta_y]$ be a real functional dependent on some parameters and on the new fluctuating fields $\eta_y$. The field $\eta_y$ is related to $\xi_x$ by the functional transformation U dependent on the parameters $\{t\}$

$$\eta_y = U_t(y,\xi_x); \quad \xi_x = U_t^{-1}(x,\eta_y). \tag{12}$$

Let us suppose that the Jacobian of the transformation (12)

$$J \equiv J(\eta,t) = \operatorname{Det}[\frac{\delta\xi_x}{\delta\eta_y}] \tag{13}$$

is a non-negative functional of $\eta_y$ for all values of the parameters $\{t\}$. The indices $x, y$ include the variables on which the fields $\xi$ and $\eta$ depend as well as the index numbering the different components of these fields. For example, we can have $x=(R_f, \tau, j)$, where $R_f$ is the coordinate of the lattice point f (if we consider a lattice), $\tau$ is Matsubara's imaginary time (for quantum systems) $0 \le \tau \le \beta$ and $j=1,\dots,s$, where s is the number of independent fluctuation fields in the system.

We have:

$$Z = \int \mathfrak{D}\xi\, e^{-\Phi(\xi)} = \int \mathfrak{D}\xi\, e^{-\Phi(\xi)+\psi(\eta)-\psi(\eta)} =$$

$$= \int \mathfrak{D}\eta\, J\, e^{-\Phi[\xi(\eta)]+\psi(\eta)-\psi(\eta)} \ge e^{-<\Phi-\psi>} \int \mathfrak{D}\eta\, e^{-\psi} J \equiv Z_t(\psi), \tag{14}$$

where

$$<\dots> = \frac{\int e^{-\psi} \dots J\mathfrak{D}\eta}{\int e^{-\psi} J\mathfrak{D}\eta},$$

$$F \le -\theta \ln Z_t(\psi).$$

Minimizing the right-hand side of the obtained inequality with respect to the parameters appearing in $\psi$ and $\{t\}$, we obtain a system of equations determining those parameters:

$$<<\delta\psi \cdot (\Phi-\psi)>> = 0,$$

$$<<(\psi-\Phi) \cdot \frac{\partial \ln J}{\partial t}>> = <\frac{\partial}{\partial t}(\ln J - \Phi)>, \tag{15}$$

where $\delta\psi$ is the variation of functional $\psi$ with respect to the parameters on which it depends, and

$$<<A \cdot B>> = <AB> - <A><B>.$$

Equations (15) allow one to determine the optimals (in the sense of best approximation to free energy) $\psi$ and $U_t$. Then the partition function is determined by the right-hand side of (14) where $\psi$ and $\{t\}$ are the solutions of (15). In this approximation the correlators are given by the expressions:

$$\frac{\int \mathfrak{D}\xi\, \xi_{x_1} \dots \xi_{x_n} e^{-\Phi}}{\int \mathfrak{D}\xi\, e^{-\Phi}} = \frac{\int \mathfrak{D}\eta\, J\, U^{-1}(x_1, \eta) \dots U^{-1}(x_n, \eta) e^{-\psi}}{\int \mathfrak{D}\eta\, e^{-\psi}}. \tag{16}$$

We call this approach to calculate the thermodynamical quantities and the correlation functions, functional analog of the variational method of Bogolubov.

4. Let's consider some possible examples of field transformations (12).

A) Linear transformation

$$\xi_x = \int t(x, y)\,\eta_y\,dy + \tilde{\epsilon}_x \quad . \tag{17}$$

In this case

$$J = \det[t(x, y)] = e^{\,\mathrm{Sp}\,\ln[t(x,y)]} = e^{\int \ln t(k)dk} \quad . \tag{18}$$

The last inequality holds if: $t(x,y)=t(x-y)$ and $t(k)=\int t(x)e^{ikx}dx$. Note that in this case the Jacobian does not depend on $\eta_y$ and the second equation of (15) becomes: $\frac{\partial \ln J}{\partial t} = <\frac{\partial \Phi}{\partial t}>$.

B) A nonlinear transformation

$$\xi_x = C(x)\,\eta_x^{2n+1} + \tilde{\xi}_x\,;\; n = 0, \pm 1, \pm 2, \ldots, C(x) > 0. \tag{19}$$

In this case

$$\frac{\delta \xi_x}{\delta \eta_y} = C(x)(2n+1)\eta_x^{2n}\,\delta(x-y)\,;\; J = e^{\int dx \ln[C(x)(2n+1)\eta_x^{2n}]} . \tag{20}$$

C) Transformation of the coordinates on which fields depend, (for example, scale transformation)

$$x \to y = t(x);\quad \xi_x = \eta_t(x),$$

$$\frac{\delta \xi_y}{\delta \eta_y} = \delta[t(x) - y]\,;\; J = \exp[-\int dx \ln \frac{dt(x)}{dx}]. \tag{21}$$

In all cases when we deal with functions of operators, we define them in a constructive way(see (8)).This means that we have an operator U which can be represented by a diagonalizable matrix and a function of U is defined by the diagonal matrix whose elements are the values of the function at the eigenvalues of U. In all applications the operator appears under the symbol "Sp" so the particular form of U in a given representation doesn't matter.

We must look for the solutions $\psi$ and $\{t\}$ of (15) in a certain class of functionals. The functional integrals appearing in (15) are calculable if, for example, $\psi$ has the form

$$\psi(\eta) = \int dy\, \psi_y\, (\eta_y). \tag{22}$$

The simplest example of this class is the Gaussian functional

$$\psi(\eta) = \frac{1}{2} \int dy\, G_y^{-1} |\eta_y|^2 .$$

The calculation of averages with a Gaussian functional can be performed using the functional analog of Wick's theorem (see (4,5)). For example

$$<\eta_{y_1} \eta_{y_2}> = G_{y_1} \delta(y_1 + y_2),$$

$$<\eta_{y_1} \eta_{y_2} \eta_{y_3} \eta_{y_4}> = G_{y_1} G_{y_3} \delta(y_1 + y_2) \delta(y_3 + y_4) + G_{y_1} G_{y_2} \delta(y_1 + y_3) \times$$
$$\times \delta(y_2 + y_4) + G_{y_1} G_{y_2} \delta(y_1 + y_4) \delta(y_2 + y_3).$$

In the case of Gaussian functional $\psi$ and supposing that the Jacobian J doesn't depend on $\eta$, the first of equations (15) becomes an equation determining by $G_y$

$$G_y = <<\Phi ; |\eta_y|^2>> . \tag{23}$$

The simplest generalization of the Gaussian functional is:

$$\psi = \sum_y [a_y |\eta_y|^2 + \Gamma_y |\eta_y| ]. \tag{24}$$

The partition function of model (24) can be calculated exactly:

$$Z(\psi) = \int \mathfrak{D}\eta\, e^{-\psi[\eta]} = \exp \sum_y \ln\{ (\frac{\pi^3}{4\Gamma_y})^{1/2} e^{\lambda_y^2} [1 - \mathrm{erf}\lambda_y]\}, \tag{25}$$

$$\lambda_y = \frac{a_y}{\sqrt{2\Gamma_y}}; \quad \mathrm{eRf}\, x = \frac{2}{\sqrt{\pi}} \int_0^x dt\, e^{-t^2} .$$

The simplest correlators have the form:

$$\phi_n(y) \equiv \frac{\int \mathfrak{D}\eta\, \mathfrak{D}\eta^* |\eta_y|^{2n} e^{-\psi[\eta]}}{\int \mathfrak{D}\eta\, \mathfrak{D}^*\eta\, e^{-\psi[\eta]}} = (\frac{-1}{\sqrt{2\Gamma_y}})^n \frac{1}{\phi(\lambda_y)} \frac{\partial^n \phi(\lambda_y)}{\partial \lambda_y^n} , \tag{26}$$

where

$$\phi(\lambda) = e^{\lambda^2}\{1 - \mathrm{erf}\lambda\}.$$

Using $\phi_n(y)$ it is easy to obtain expressions for other correlators. We introduce generalized Kroenecker's symbol

$$\delta(y_1, \dots, y_n) = \begin{cases} 1 & |y_1| = |y_2| = \dots = |y_n|; \quad y_1 + \dots + y_{2n} = 0 \\ 0 & \text{on other cases.} \end{cases} \tag{27}$$

Then

$$\langle \eta_{y_1} \eta_{y_2} \rangle = \phi_1(y_1)\delta(y_1, y_2)$$

$$\langle \eta_{y_1} \dots \eta_{y_4} \rangle = \phi_2(y_1)\delta(y_1, \dots, y_4) + [1 - \delta(y_1, y_2, y_3)] \times$$

$$\times [\phi_1(y_1)\phi_1(y_3)\delta(y_1, y_2)\delta(y_3, y_4) + 2 \text{ permutation terms} \tag{28}$$

$$\langle \eta_{y_1}, \dots, \eta_{y_6} \rangle = \phi_3(y_1)\delta(y_1 \dots y_6) + [1 - \delta(y_1, \dots, y_6)] \times$$

$$\times \phi_2(y_1)\phi_2(y_5)\delta(y_1, \dots, y_4)\delta(y_5, y_6) + 14 \text{ permutation terms} +$$

$$+ [1 - \delta(y_1, \dots, y_6)][1 - \delta(y_1, \dots, y_4)][1 - \delta(y_2, \dots, y_5)] \times$$

$$+ \phi_1(y_1)\phi_1(y_3)\phi_1(y_5)\delta(y_1, y_2)\delta(y_3, y_4)\delta(y_5, y_6) +$$

$$+ 14 \text{ permutation terms, etc.}$$

Let's now apply this variational method to some simple models.

a) Let the functional $\Phi$ have the form

$$\Phi(\xi) = \sum_{n=1}^{\infty} \Phi_{2n}(\xi); \; \Phi_{2n} = \frac{1}{(2n)!} \int d\bar{k}_1 \dots d\bar{k}_{2n} \delta(\bar{k}_1 + \dots + \bar{k}_{2n}) u_{2n} \xi_{\bar{k}_1} \dots \xi_{\bar{k}_{2n}}. \tag{29}$$

Here $\bar{k}$ has the meaning of the wave vector and $0 \le k \le k_0$.

We suppose also that $u_{2n}(\bar{k}_1, \bar{k}_2, \dots, \bar{k}_{2n-1}, \bar{k}_{2n})$ is a positive symmetric function of $\bar{k}_1, \dots, \bar{k}_{2n}$ and that the series $\sum_{n=1}^{\infty} \frac{u_{2n}}{(2n-2)!!} x^{2n}$ converges uniformly with respect to $\bar{k}_1, \dots, \bar{k}_{2n}$ in the interval $-a \le x \le a$. We take the trial functional $\psi[\eta]$ of Gaussian type:

$$\psi[\eta] = \frac{1}{2} \int d\bar{k}\, G_{\bar{k}}^{-1} |\eta_{\bar{k}}|^2 \qquad \xi_{\bar{k}} = \eta_{\bar{k}} .$$

Then from (15) we obtain an integral nonlinear equation for $G_{\bar{k}}$

$$G_{\bar{k}}^{-1} = \sum^{\infty} \frac{1}{(2n-2)!!} \int d\bar{k}_1 d\bar{k}_3^{-0} \dots d\bar{k}_{2n-3}\, u_{2n}(\bar{k}_1, -\bar{k}_1, \dots, \bar{k}_{2n-3}, -\bar{k}_{2n-3}, \bar{k}, -\bar{k}) \times \tag{30}$$

$$\times\, G(\bar{k}_1) G(\bar{k}_3) \dots G(\bar{k}_{2n-3}).$$

In the particular case when (model $\xi^4$)

$$\Phi(\xi) = \frac{1}{2} \int dk\, (\tau + k^2) |\xi_{\bar{k}}|^2 + \frac{u}{4} \int d\bar{k}_1 d\bar{k}_2 d\bar{k}_3 \xi_{\bar{k}} \xi_{\bar{k}} \xi_{\bar{k}}\ \xi_{-\bar{k}_1 - \bar{k}_2 - \bar{k}_3} ,$$

we have $G_{\bar{k}}^{-1} = \tau + k^2 + \Delta$, where $\Delta$ is determined by the equation

$$\Delta = +2\pi u [k_0 - \sqrt{\tau + \Delta}\, \mathrm{arc\,tg} \frac{k_0}{\sqrt{\tau + \Delta}}] .$$

and for the critical temperature, determined from the condition $G_{k=0}^{-1}(T_c) = 0$, we obtain in this approximation

$$\tau(T_c) = -2\pi k_0 u .$$

b) Let's apply the method to the model $\xi^4$

$$\Phi(\xi) = \frac{1}{2} \Sigma (\tau + k^2) |\xi_{\bar{k}}|^2 + \frac{u}{v} \sum_{\bar{k}_1 \bar{k}_2 \bar{k}_3} \xi_{\bar{k}_1} \xi_{\bar{k}_2} \xi_{\bar{k}_3}\ \xi_{-\bar{k}_1 - \bar{k}_2 - \bar{k}_3} \tag{31}$$

using the trial functional

$$\psi = \frac{1}{2} \sum_{\bar{k}} r(\bar{k}) |\xi_{\bar{k}}|^2 + a(\bar{k}) |\xi_{\bar{k}}|^4 \tag{32}$$

with $r(k) = \tau + k^2$. Equation (15) determining $a(k)$ has the form

$$\langle\langle |\xi_{\bar{k}}|^4 , (\Phi - \psi) \rangle\rangle_{\psi} = 0, \tag{33}$$

using (26-28) we obtain

$$a(k) = 12u\,F(k) \int \frac{d^3p}{(2\pi)^3}\phi_1(p) \tag{34}$$

where $F(k) = \dfrac{\phi_3(k) - \phi_2(k)\phi_1(k)}{\phi_4(k) - \phi_2^2(k)}$ and the $\phi_n$ are defined in (26). In the critical point we have $\phi_1^{-1}(0,T_c) = 0$ and

$$r(T_c) = -12u \int \frac{d^3k}{(2\pi)^3}\phi_1(k,T_c), \tag{35}$$

For $T \approx T_c$ and small $\vec{k}$

$$\phi_1(\bar{k},T) = \frac{1}{2}\,\frac{1}{k^2+\lambda^2}, \tag{36}$$

where

$$\lambda^2 = r(T) + 12u \int \frac{d^3\bar{k}}{(2\pi)^3}\phi_1(\bar{k},T). \tag{37}$$

Using those formulae we obtain for the critical indices the values $\alpha = 0$, $\beta = 1/2$, $\gamma = 2$, $\delta = 5$, $\eta = 0$, $\nu = 1$ (in the usual notation) and for the critical temperature

$$r(T_c) = -\frac{3uk_0}{\pi}.$$

These examples, of course, only illustrate the method developed in this paper. Nevertheless, we think that its application will allow us to go out of the frames of mean field theory in some complicated models of statistical mechanics (magnetism [11,12], liquid crystals [13]). On the other hand it appears interesting to use the functional [32] in the Wilson renormalization group approach to the theory of critical phenomena.

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