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V.I.Yukalov

RENORMALIZATION OF QUASI-HAMILTONIANS UNDER HETEROPHASE AVERAGING

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The theory of heterophase fluctuations developed by the author [1-3] is essentially based on the notion of an effective Hamiltonian. The latter appears after a summation over heterophase fluctuations [2-4] in the partition function like a renormalized Hamiltonian appears after summing a part of variables in the renormalization group method [5,6]. The system with heterophase fluctuations is generally nonequilibrium, it is quasi-equilibrium. Its most logical description presupposes the use of the quasi-equilibrium Gibbs ensemble whose statistical operator contains a quasi-Hamiltonian in place of a Hamiltonian. In paper [7] a heterophase ensemble consisting of a set of quasi-equilibrium ensembles with various phase configurations has been constructed, and it has been shown how to calculate the corresponding thermodynamic potential. However, solely one question is yet undetermined - how to define in a correct way mathematical expectations for the operators of observables when averaging over this heterophase quasi-equilibrium ensemble. An answer to this question is given in the present paper. The succession of actions is formulated in the abstract.

Consider the system of particles on the Lebesgue measurable manifold $\mathbb{V} = \{ x \,|\, \mathrm{mes}\, \mathbb{V} = \int_{\mathbb{V}} dx = V \}$. A Hilbert space $\mathcal{H}$ of microscopic states is given on the manifold $\mathbb{V}$. The algebra of local observables $\mathcal{A}(\Lambda) = \{ A(\Lambda) \}$ $(\Lambda \subset \mathbb{V})$ is defined in the space $\mathcal{H}$; this algebra being composed by operators of the form

$$A(\Lambda) = \sum_k \int_\Lambda A_k(x_1, x_2, \ldots x_k)\, dx_1\, dx_2 \ldots dx_k ,$$

where $A_k(\ldots)$ is an operator distribution and $A_0 \equiv \mathrm{const} \cdot \hat{1}$. Constructing an ordered manifold $\{ \Lambda_i \,|\, i = 1, 2, \ldots \}$ of bounded open regions $\Lambda_i \subset \Lambda_{i+1}$ and an isotonic sequence of algebras $\mathcal{A}(\Lambda_1) \subset \mathcal{A}(\Lambda_2) \subset \ldots$, in which $\Lambda_1 \subset \Lambda_2 \subset \ldots$, one obtains a net of algebras $\{ \mathcal{A}(\Lambda_i) \}$. For a net of algebras an inductive limit can be defined [8], called a quasi-local algebra.

Suppose the considered system consists of several thermodynamic phases, enumerated by the index $\alpha = 1, 2, \ldots 5$. The separation of phases in the real space is characterized by a family of submanifolds $\{\mathbb{V}_\alpha\}$ forming a covering of the manifold $\mathbb{V}$,

$$\bigcup_{\alpha=1}^{s} \mathbb{V}_\alpha = \mathbb{V}, \quad \sum_{\alpha=1}^{s} V_\alpha = V \quad (V_\alpha \equiv \mathrm{mes}\, \mathbb{V}_\alpha). \tag{1}$$

In its turn, in the space $\mathcal{H}$ of microscopic states one is able [7,9] to separate subspaces $\mathcal{F}_\alpha \subset \mathcal{H}$ $(\alpha = 1, 2, \ldots s)$, such that a conditional probability measure corresponding to the thermodynamic phase α is concentrated on the subspace $\mathcal{F}_\alpha$. Each of spaces $\mathcal{F}_\alpha$ is a set of vectors that are typical [10] for the phase α. The representation $\pi_\alpha[\mathcal{A}(\Lambda_\alpha)]$ of the algebra of local observables for the regions $\Lambda_\alpha \subset \mathbb{V}_\alpha$ is defined on the space $\mathcal{F}_\alpha$. Writing down the representations of the operators from this algebra one can define the operator distributions $A_{k\alpha}(\ldots)$ by the equality

$$\pi_\alpha[A(\Lambda_\alpha)] = \sum_k \int_{\Lambda_\alpha} A_{k\alpha}(x_1, x_2, \ldots x_k)\, dx_1 dx_2 \ldots dx_k. \tag{2}$$

To divide the manifold $\mathbb{V}$ into a set of submanifolds $\{\mathbb{V}_\alpha\}$, one may use the Gibbs method of separating surfaces [11] in his theory of heterogeneous systems. Mathematically, it is convenient [3,4,7] to produce such a division by fixing a set of characteristic functions of submanifolds,

$$\xi_\alpha(x) = \begin{cases} 1, & x \in \mathbb{V}_\alpha, \\ 0, & x \notin \mathbb{V}_\alpha. \end{cases} \tag{3}$$

Then, invoking the identity

$$\int_{\mathbb{V}_\alpha} A_{k\alpha}(x_1, \ldots x_k)\, dx_1 \ldots dx_k \equiv \int_{\mathbb{V}} A_{k\alpha}(x_1, \ldots x_k; \xi_\alpha)\, dx_1 \ldots dx_k,$$

the representation of the quasi-local algebra, $\pi_\alpha[\mathcal{A}(\mathbb{V}_\alpha)]$, can be extended to the representation of a quasi-local algebra, $\pi_\alpha[\mathcal{A}(\mathbb{V}; \xi_\alpha)] \equiv \mathcal{A}_\alpha(\xi_\alpha)$ with the operator distributions

$$A_{k\alpha}(x_1, x_2, \ldots x_k; \xi_\alpha) = A_{k\alpha}(x_1, x_2, \ldots x_k) \prod_{j=1}^{k} \xi_\alpha(x_j).$$

As is clear, the function $\xi_\alpha(x)$ plays the role of an additional functional variable. In order to define a representation of the

quasi-local algebra $\mathcal{A}(\mathbb{V})$, that could be called a global algebra as distinct from the quasi-local algebras, consider $\mathcal{F}_\alpha$.

Suppose that there exists a topological space $\mathcal{F}$, on which a mapping $map_\alpha : \mathcal{F} \to \mathcal{F}_\alpha$ is given. The three $(\mathcal{F}, map_\alpha, \mathcal{F}_\alpha)$ is called the fiber space, $\mathcal{F}$ is the total space, $\mathcal{F}_\alpha$ is the fiber base [12]. The procedure of obtaining $\mathcal{F}_\alpha$ from $\mathcal{F}$ by means of map_α is called fibering, and the inverse process of reconstructing $\mathcal{F}$ out of $\mathcal{F}_\alpha$ is a fiber section. When the total spaces of different fiberings are homeomorphic and their bases are the same, then such fiberings are equivalent. For our purpose any of equivalent fiberings may be used. It is convenient to choose the so-called standard fibering with the total space as a tensor product $\bigotimes_\alpha \mathcal{F}_\alpha$. This total space under a fixed set of mappings $\mathcal{F} \to \mathcal{F}_\alpha$ $(\alpha = 1, 2, \ldots s)$ should be called the standard fiber space

$$\mathcal{F} = \bigotimes_\alpha \mathcal{F}_\alpha \qquad (map_\alpha : \mathcal{F} \to \mathcal{F}_\alpha). \tag{4}$$

Fiber bases corresponding to different thermodynamic phases are not necessarily mutually orthogonal, although in many cases it is so [9].

Thus, the global algebra $\mathcal{A}(\mathbb{V})$ is to be interpreted as a direct sum of quasi-local algebras $\mathcal{A}(\mathbb{V}; \xi_\alpha)$, and its representation $\pi[\mathcal{A}(\mathbb{V})] \equiv \mathcal{A}(\xi)$, where

$$\xi \equiv \{\xi_\alpha(x) \mid \alpha = 1, 2, \ldots s;\ x \in \mathbb{V}\}, \tag{5}$$

has to be defined on the standard fiber space (4) in the form

$$\mathcal{A}(\xi) = \bigoplus_\alpha \mathcal{A}_\alpha(\xi_\alpha) = \{A(\xi)\}. \tag{6}$$

The representations of operators have the structure

$$A(\xi) = \bigoplus_\alpha A_\alpha(\xi_\alpha),$$

$$A_\alpha(\xi_\alpha) = \sum_k \int_{\mathbb{V}} A_{k\alpha}(x_1, x_2, \ldots x_k) \prod_{j=1}^{k} \xi_\alpha(x_j)\, dx_j. \tag{7}$$

The many of all possible collections of ξ form the topological space $\{\xi\}$, on which a functional measure $\mathcal{D}\xi$ can be given [7]. The statistical operator of a quasi-equilibrium heterophase ensemble is presentable as

$$\rho(\xi) = e^{-\Gamma(\xi)} \Big/ \mathrm{Tr}_{\mathcal{F}} \int e^{-\Gamma(\xi)}\, \mathcal{D}\xi, \tag{8}$$

where $\Gamma(\xi)$ is a quasi-Hamiltonian of the system. Mathematical expectations answering observable quantities are defined by the formula

$$< A > = \underset{\mathcal{F}}{\mathrm{Tr}} \int \rho(\xi)\, A(\xi)\, \mathcal{D}\xi \ . \tag{9}$$

Functional integrals in eqs. (8) and (9) describe the averaging over phase configurations.

Introducing the functional measure $\mathcal{D}\xi$ one is able to note that the averaging over phase configurations contains two kinds of actions. The first one deals with all possbile configurations under a fixed set $p \equiv \{p_\alpha \mid \alpha = 1, 2, \dots s\}$ of geometrical probabilities

$$p_\alpha = \frac{V_\alpha}{V} \qquad \left(0 \le p_\alpha \le 1 \ , \ \sum_{\alpha=1}^{s} p_\alpha = 1 \right) . \tag{10}$$

The second action is the variation of each p_α from zero to unity taking account of their normalization. In correspondence to these actions

$$\mathcal{D}\xi = \mathcal{D}_p \xi \, dp \ , \quad dp = \delta\left(\sum_{\alpha=1}^{s} p_\alpha - 1 \right) \prod_{\alpha=1}^{s} dp_\alpha \ . \tag{11}$$

The functional differential $\mathcal{D}_p\xi$ is defined in the following manner. One divides each of submanifolds $\mathbb{V}_\alpha$ by means of subcoverings $\{\mathbb{V}_{\alpha i}\}$ so that

$$\bigcup_{i=1}^{n_\alpha} \mathbb{V}_{\alpha i} = \mathbb{V}_\alpha \ , \ \sum_{i=1}^{n_\alpha} V_{\alpha i} = V_\alpha \qquad \left(\sum_{\alpha=1}^{s} n_\alpha = n \ , \ V_{\alpha i} \equiv mes\, \mathbb{V}_{\alpha i} \right) .$$

The characteristic function (3) is presentable as the sum

$$\xi_\alpha(x) = \sum_{i=1}^{n_\alpha} \xi_{\alpha i}(x - a_{\alpha i}) \ , \ \xi_{\alpha i}(x - a_{\alpha i}) = \begin{cases} 1, & x \in \mathbb{V}_{\alpha i} \ , \\ 0, & x \notin \mathbb{V}_{\alpha i} \ , \end{cases}$$

in which $a_{\alpha i} \in \mathbb{V}_{\alpha i}$. Implying the limiting transition

$$n \to \infty \ , \ n_\alpha \to \infty \ , \ V_{\alpha i} \to 0 \qquad (p_\alpha = const) \ , \tag{12}$$

one can write the asymptotic expression

$$\mathcal{D}_p \xi \simeq \prod_{\alpha=1}^{s} \prod_{i=1}^{n_\alpha} \frac{da_{\alpha i}}{V} \qquad (n \to \infty) \ . \tag{13}$$

Finally, the averaging of a functional $F(\xi)$ over phase configurations under a fixed set of geometric probabilities (10) is defined as the functional integral

$$\int F(\xi)\, \mathcal{D}_p \xi = \lim_{n \to \infty} \int F(\xi) \prod_{\alpha=1}^{s} \prod_{i=1}^{n_\alpha} \frac{da_{\alpha i}}{V} \ , \tag{14}$$

in which the limit means eq.(12).

<u>Theorem 1.</u> If the functional $F(\xi)$ is a polynomial in characteristic functions (3), then

$$\int F(\xi)\, \mathcal{D}_p \xi = F(p) \ , \tag{15}$$

where $F(p)$ follows from $F(\xi)$ as a result of the replacement $\xi_\alpha(x) \to p_\alpha$.

Proof with all details has been given in ref. [7] .

<u>Corollary.</u> The theorem can be spread to arbitrary functionals presentable as series in powers of characteristic functions of submanifolds if to implicate, as it is usually supposed in physical problems, that summation and integration can be interchanged. Then formula (9) for a mathematical expectation leads to

$$< A > = \underset{\mathcal{F}}{\mathrm{Tr}} \int_0^1 \rho(p)\, A(p)\, dp \ , \tag{16}$$

where the differential dp is defined in eq.(11), and

$$\rho(p) = e^{-\Gamma(p)} \Big/ \underset{\mathcal{F}}{\mathrm{Tr}} \int_0^1 e^{-\Gamma(p)} dp \ . \tag{17}$$

<u>Theorem 2.</u> Let the function

$$y(p) = -\frac{1}{N} \ln \underset{\mathcal{F}}{\mathrm{Tr}}\, e^{-\Gamma(p)} \ , \tag{18}$$

in which $N \equiv N(V)$ is a number such that

$$N \to \infty \ , \ V \to \infty \ , \ N/V \to const \ , \tag{19}$$

has an absolute minimum

$$y(w) = \mathrm{abs}\min_{p} y(p) \qquad \left(w \equiv \{w_\alpha \,|\, \alpha = 1, 2, \dots s\}\right). \tag{20}$$

Then

$$\lim_{N\to\infty} \frac{1}{N} \mathop{\mathrm{Tr}}_{\mathcal{F}} \left[\int_0^1 \rho(p) A(p)\, dp - \rho(w) A(w) \right] = 0 , \tag{21}$$

where the limit is understood in the sense of eq. (19), and

$$\rho(w) = e^{-\Gamma(w)} \Big/ \mathop{\mathrm{Tr}}_{\mathcal{F}} e^{-\Gamma(w)} . \tag{22}$$

<u>Proof.</u> Introducing the notation

$$\bar{A}(p) \equiv \mathop{\mathrm{Tr}}_{\mathcal{F}} e^{-\Gamma(p)} A(p) \Big/ \mathop{\mathrm{Tr}}_{\mathcal{F}} e^{-\Gamma(p)}$$

and using eq. (18), one can write down

$$\mathop{\mathrm{Tr}}_{\mathcal{F}} \rho(p) A(p) = e^{-Ny(p)} \bar{A}(p) \Big/ \int_0^1 e^{-Ny(p)} dp .$$

Applying the Laplace method as $N \to \infty$, we find

$$\int_0^1 e^{-Ny(p)} \bar{A}(p)\, dp \simeq e^{-Ny(w)} \bar{A}(w) \prod_{\alpha=1}^{s-1} \left(\frac{2\pi}{N y''_\alpha} \right)^{1/2} ,$$

where $y''_\alpha \equiv \partial^2 y(w)/\partial w_\alpha^2 \quad (N \to \infty)$. Therefore,

$$\mathop{\mathrm{Tr}}_{\mathcal{F}} \int_0^1 \rho(p) A(p)\, dp \simeq \bar{A}(w) .$$

Remembering the notation for $\bar{A}(p)$ and definition (22), we obtain (21).

<u>Corollary.</u> The mathematical expectation (16) becomes

$$\langle A \rangle \simeq \mathop{\mathrm{Tr}}_{\mathcal{F}} \rho(w) A(w) \qquad (V \to \infty) . \tag{23}$$

The representation of operators (7) of observables on the fiber space (4) takes the structure

$$A(w) = \bigoplus_\alpha A_\alpha(w_\alpha) ,$$
$$A_\alpha(w_\alpha) = \sum_k w_\alpha^k \int_{\mathbb{V}} A_{k\alpha}(x_1, x_2, \dots x_k)\, dx_1 dx_2 \dots dx_k . \tag{24}$$

The set $w \equiv \{w_\alpha\}$ defines the probabilities of thermodynamic phases and is to be found from the minimization of the thermodynamic potential

$$y(w) = -\frac{1}{N} \ln \mathop{\mathrm{Tr}}_{\mathcal{F}} e^{-\Gamma(w)} \tag{25}$$

under the normalization condition $\sum_{\alpha=1}^{s} w_\alpha = 1$ following from eq.(10).

To concretize the approach developed above, consider a system with the Hamiltonian in the Heisenberg representation

$$H(\Lambda) = \int_\Lambda H_1(x)\, dx + \int_\Lambda H_2(x, x')\, dx\, dx' ,$$
$$H_1(x) = \psi^+(x) \left[-\frac{\nabla^2}{2m} + U(x) \right] \psi(x) , \tag{26}$$
$$H_2(x, x') = \frac{1}{2} \psi^+(x) \psi^+(x') \Phi(x, x') \psi(x') \psi(x) .$$

Operator distributions $H_{1\alpha}(x)$ and $H_{2\alpha}(x, x')$ can be defined by rule (2) when introducing the representation of operator (26) on the space $\mathcal{F}_\alpha$. Representations of the algebra of field operators could be constructed in a perfect analogy with the construction of the representations of the algebra of local observables. For the field operator $\psi(f) = \int_{\mathbb{V}} f(x) \psi(x)\, dx$, in which $f(x)$ is any square-integrable function, one sets the representation $\pi_\alpha[\psi(f)]$ on the space $\mathcal{F}_\alpha$. In its turn, this representation defines the operator distribution $\psi_\alpha(x)$ with the help of relations

$$\pi_\alpha[\psi(f)] = \int_{\mathbb{V}_\alpha} f(x) \psi_\alpha(x)\, dx = \int_{\mathbb{V}} f(x) \psi_\alpha(x) \xi_\alpha(x)\, dx . \tag{27}$$

The representation of the operator $H(\mathbb{V})$ on the fiber space (4) according to (7), has the form

$$H(\xi) = \bigoplus_{\alpha} H_{\alpha}(\xi_{\alpha}),$$

$$H_{\alpha}(\xi_{\alpha}) = \int_{\mathbb{V}} H_{1\alpha}(x)\xi_{\alpha}(x)\,dx + \int_{\mathbb{V}} H_{2\alpha}(x,x')\xi_{\alpha}(x)\xi_{\alpha}(x')\,dx\,dx'. \tag{28}$$

The partition of the manifold $\mathbb{V}$ into submanifolds $\mathbb{V}_{\alpha}$ occupied by different thermodynamic phases by no means presupposes the uniformity of these phases. These phases as a whole are already nonuniform if only due to the existence of interphase transition layers. The Gibbs dividing surface [11] presents a conditional geometric boundary placed somewhere inside a transition layer. The measured thermodynamic quantities can be defined so that they do not depend on a position of the dividing surface. Imposing some additional limitations, e.g. the equimolecularity condition [11], one may fix the dividing surface in a macroscopically unique manner. In our case an ambiguity of choosing separting surfaces is not at all important as far as we average over all their possible positions.

A nonuniform system consisting of several thermodynamic phases is quasi-equilibrium [7]. Consequently, in the same fashion as for any locally equilibrium system [13], the local quantities must have a meaning, such as the local energy density

$$e_{\alpha}(x;\xi_{\alpha}) = \operatorname*{Tr}_{\mathcal{F}} \rho(\xi) H_{\alpha}(x;\xi_{\alpha}), \tag{29}$$

$$H_{\alpha}(x;\xi_{\alpha}) = H_{1\alpha}(x)\xi_{\alpha}(x) + \int_{\mathbb{V}} H_{2\alpha}(x,x')\xi_{\alpha}(x)\xi_{\alpha}(x')\,dx'$$

and the local number-of-particle density

$$n_{\alpha}(x;\xi_{\alpha}) = \operatorname*{Tr}_{\mathcal{F}} \rho(\xi) N_{\alpha}(x;\xi_{\alpha}),$$

$$N_{\alpha}(x;\xi_{\alpha}) = N_{\alpha}(x)\xi_{\alpha}(x), \quad N_{\alpha}(x) = \psi_{\alpha}^{+}(x)\psi_{\alpha}(x). \tag{30}$$

The statistical operator is given by formula (8) from which the normalization is evident

$$\operatorname*{Tr}_{\mathcal{F}} \int \rho(\xi)\,\mathcal{D}\xi = 1. \tag{31}$$

Expression (8) contains a yet unknown quasi-Hamiltonian $\Gamma(\xi)$.

An explicit form of the quasi-Hamiltonian can be found by demanding that the entropy

$$S = -\operatorname*{Tr}_{\mathcal{F}} \int \rho(\xi)\ln\rho(\xi)\,\mathcal{D}\xi \tag{32}$$

be maximal with respect to variations of $\rho(\xi)$ under conditions (29)-(31). This yields

$$\Gamma(\xi) = \bigoplus_{\alpha} \Gamma_{\alpha}(\xi_{\alpha}),$$

$$\Gamma_{\alpha}(\xi_{\alpha}) = \int_{\mathbb{V}} \beta_{\alpha}(x,\xi_{\alpha})\left[H_{\alpha}(x;\xi_{\alpha}) - \mu_{\alpha}(x,\xi_{\alpha})N_{\alpha}(x;\xi_{\alpha})\right]dx, \tag{33}$$

where the inverse temperature $\beta_{\alpha}(x,\xi_{\alpha})$ and the chemical potential $\mu_{\alpha}(x,\xi_{\alpha})$ play the role of the Lagrange multipliers, ensuring the nonuniformity of a system corresponding to a given choice of separating surfaces.

After averaging over phase configurations the renormalized quasi-Hamiltonian $\Gamma(w)$ entering into the statistical operator (22) assumes the form

$$\Gamma(w) = \bigoplus_{\alpha} \Gamma_{\alpha}(w_{\alpha}),$$

$$\Gamma_{\alpha}(w_{\alpha}) = w_{\alpha}\int_{\mathbb{V}} \beta_{\alpha}(x)\left[H_{1\alpha}(x) - \mu_{\alpha}(x)N_{\alpha}(x)\right]dx + {}$$

$$+ w_{\alpha}^{2}\int_{\mathbb{V}} \beta_{\alpha}(x)H_{2\alpha}(x,x')\,dx\,dx', \tag{34}$$

in which the renormalized quantities

$$\beta_{\alpha}(x) = \langle \beta_{\alpha}(x,\xi_{\alpha})\rangle, \quad \mu_{\alpha}(x) = \langle \mu_{\alpha}(x,\xi_{\alpha})\rangle \tag{35}$$

figure as functions defining the taken heterophase ensemble. Each of renormalized quasi-Hamiltonians $\Gamma_{\alpha}(w_{\alpha})$ corresponds not to a sole part of a real system, occupied by the phase α, but to an abstract system representing an averaged infinite many of spatially nonuniform subsystems taking arbitrary shapes and sizes, and having the properties of the thermodynamic phase α. Such an averaged abstract many can be called the phase replica [7]. Emphasize that the renormalized quasi-Hamiltonian (34) retains an information about the presence of transition layers and a corresponding surface energy [7].

Let there be no external fields acting on the considered system so that a stationary separation of phases could occur. That is the appearance of nuclei of different competing phases is a purely fluctuational process. The quasi-equilibrium system with such heterophase fluctuations serves as an example of self-optimizing systems [14]. When all phases and all parts of the system are in equal external conditions, then the average quantities (35) characterizing these conditions have to be constant:

$$\beta_\alpha(x) = \beta \; , \quad \mu_\alpha(x) = \mu \; . \tag{36}$$

Equalities (36) showing that in the system there is a heterophase equilibrium on the average can be called the equilibrium condition for phase replicas [7]. Eqs. (36) being true, the renormalized Hamiltonian (34) becomes

$$\Gamma(w) = \beta \widetilde{H} \; , \quad \widetilde{H} = \bigoplus_\alpha H_\alpha \; ,$$
$$H_\alpha = w_\alpha \int_{\mathbb{V}} \psi_\alpha^+(x)\left[-\frac{\nabla^2}{2m} + U(x) - \mu\right]\psi_\alpha(x)\, dx \; +$$
$$+ \frac{w_\alpha^2}{2} \int_{\mathbb{V}} \psi_\alpha^+(x)\psi_\alpha^+(x')\, \Phi(x,x')\, \psi_\alpha(x')\psi_\alpha(x)\, dx\, dx' \; . \tag{37}$$

Now the mathematical expectation (23) is

$$< A > \simeq \underset{\mathcal{F}}{\mathrm{Tr}}\; \widetilde{\rho}\, \widetilde{A} \qquad (\mathbb{V} \to \infty) \tag{38}$$

which formally corresponds to an equilibrium case with the statistical operator

$$\widetilde{\rho} = e^{-\beta \widetilde{H}} \Big/ \underset{\mathcal{F}}{\mathrm{Tr}}\; e^{-\beta \widetilde{H}} \tag{39}$$

and the operator representation $\widetilde{A} \equiv A(w)$ on the fiber space (4). The renormalized chemical potential μ can be expressed in a usual way through the renormalized inverse temperature β and the average number of particles

$$N = \sum_{\alpha=1}^{s} N_\alpha \; , \quad N_\alpha = w_\alpha \int < \psi_\alpha^+(x)\, \psi_\alpha(x) > dx \; .$$

Here and in what follows $\int dx$ means the integration over the whole manifold $\mathbb{V}$.

Minimizing the thermodynamic potential (25) under the normalization condition $\sum_{\alpha=1}^{s} w_\alpha = 1$ or finding an absolute minimum of the potential $y = y(w) + \beta\lambda \sum_{\alpha=1}^{s} w_\alpha$, we get the equations for phase probabilities

$$w_\alpha = (\mu R_\alpha - K_\alpha - \lambda) / 2\Phi_\alpha \qquad (\alpha = 1, 2, \ldots s) \; , \tag{40}$$

with the Lagrange multiplier

$$\lambda = \left(\sum_{\alpha=1}^{s} \frac{\mu R_\alpha - K_\alpha}{\Phi_\alpha} - 2 \right) \Big/ \sum_{\alpha=1}^{s} \frac{1}{\Phi_\alpha}$$

and the notation

$$K_\alpha = \frac{1}{N} \int < \psi_\alpha^+(x)\left[-\frac{\nabla^2}{2m} + U(x)\right]\psi_\alpha(x) > dx \; ,$$

$$\Phi_\alpha = \frac{1}{2N} \int < \psi_\alpha^+(x)\psi_\alpha^+(x')\, \Phi(x,x')\, \psi_\alpha(x')\psi_\alpha(x) > dx\, dx' \; ,$$

$$R_\alpha = \frac{1}{N} \int < \psi_\alpha^+(x)\, \psi_\alpha(x) > dx \; .$$

The developed theory is applicable to heterophase systems of arbitrary nature and any number of thermodynamic phases. It can be even generalized to the case of a continuous phase mixture, when the phase index α runs over a continuous many $\{\alpha\}$. For example, this can have to do with magnetic phases with different local values or directions of magnetizations. Such a situation can arise in disordered matters with random interactions [15] or in random external fields [16] in the presence of a frustration [17]. It might be relevant to spin glasses [18] having a cluster structure [19,20]. The generalization to a continuous phase mixture can be done quite simply. There the fiber space (4) becomes a continuous product whose definition has been given in ref. [9]. A measure $dm(\alpha)$ on the many $\{\alpha\}$ lets us to represent the global algebra on the fiber space (4) as a direct integral on the field of representations $\{A_\alpha(\xi_\alpha)\}$, $\mathcal{A}(\xi) = \int^{\oplus} \mathcal{A}_\alpha(\xi_\alpha)\, dm(\alpha)$. All subsequent expressions retain their sense when changing the sums over α by the corresponding integrals over $dm(\alpha)$.

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Юкалов В.И. E17-87-44

Ренормировка квазигамильтонианов
при гетерофазном усреднении

Строится представление алгебры локальных наблюдаемых для гетерофазной системы. Усреднение по фазовым конфигурациям определяется как континуальное интегрирование по характеристическим функциям подмножеств. Средние от операторов наблюдаемых величин задаются с помощью ансамбля квазиравновесных ансамблей Гиббса. Находятся выражения для этих средних, преобразованные в результате гетерофазного усреднения. Это позволяет получить явный вид ренормированного квазигамильтониана. Дается обобщение подхода на случай непрерывного множества фаз.

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Yukalov V.I. E17-87-44

Renormalization of Quasi-Hamiltonians
under Heterophase Averaging

A representation of the algebra of local observables for a heterophase system is constructed. Averaging over phase configurations is defined as a functional integration over characteristic functions of submanifolds. Averages for the operators of observables are given with the use of an ensemble of the quasi-equilibrium Gibbs ensembles. Expressions for these averages, transformed as a result of the heterophase averaging, are found. This allows us to obtain an explicit form for a renormalized quasi-Hamiltonian. A generalization of the approach to the case of a continuous many of phases is made.

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

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