

Supersymmetric field theory of a nonequilibrium stochastic system as applied to disordered heteropolymers

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Abstract. A supersymmetric field-theoretical scheme is derived based on the Langevin equation, which enables memory and nonergodicity effects in a nonequilibrium stochastic system with quenched disorder to be described in an optimal manner. This scheme is applied to a disordered heteropolymer whose effective Hamiltonian is found to be simply the free energy as a function of the compositional order parameter. Instead of the Langevin equation, an effective equation of motion is used here to describe the way different monomers alternate as we move along a polymer chain. The isothermal and adiabatic susceptibilities, memory parameter, and irreversible response are determined as functions of the temperature and the intensity of quenched disorder.

1. Introduction

Traditionally, the subject matter of physics relates to inanimate nature: elementary particles, nuclei, atoms, small molecules and clusters, gases and plasmas, condensed media, astronomical objects, and the like (a review of the contemporary ‘physical minimum’ can be found in Ref. [1]). A cardinal change of the situation has occurred in the past few years, when the laws of statistical physics were applied to the

explanation of behavior of *complex systems* [2, 3]. Such systems are characterized by fractal properties, anomalous transfer phenomena, annealed relaxation, nonadditive properties, effects of self-organization, etc. [4–6]. The theory of complex systems allows the description of social phenomena like the evolution of society and breakout of wars [7], economic processes [8–10], traffic flows and flows of granular materials [11–13], and many other things [14–31].

The foundations of the theory of complex systems were laid in the seminal works [14, 15], which discovered a new object of study — *soft condensed media*. Such media constitute nonequilibrium thermodynamic systems exhibiting memory and nonergodicity effects which are determined by quenched disorder in the potential distribution of the interparticle interaction and field, conjugate to an order parameter. The most popular examples of such systems are spin glasses [16–18], the Hopfield model describing associative memory [19–21], and the like [22]. A special place in this list belongs to disordered heteropolymers, marked from the practical standpoint by the unique combination of mechanical, thermal, chemical and other properties [23–28]. This object is also exceptional among the others in the fact that it was used for the first successful application of the statistical physics of polymers to the description of complex systems [29–31]. By contrast to the theories of such systems, which are often phenomenological in nature, the theory of polymers proceeds from the microscopic approach formulated by I M Lifshitz [32].

As we know, this approach is based on the use of two large parameters. Firstly, the covalent bond energy in the polymer chain is much greater than the characteristic magnitude of

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interaction between the particles. This allows the consideration of this chain as a threadlike structure fixed by the longitudinal covalent bonds. In other words, the polymer chain possesses linear memory corresponding to quenched disorder in spin glasses. The other large parameter is the total number of monomer chain links N — for example, in synthetic polymers $N \sim 10^4 - 10^5$, and in DNA macromolecules $N \sim 10^5 - 10^7$. Accordingly, one can use the thermodynamic limit $N \rightarrow \infty$, which allows the treatment of the polymer chain using the standard methods of statistical physics [33].

As the external conditions change, the polymer systems may experience transformations of two basic types: microphase separation leading to the formation of domain structure with a mesoscopic period, and transition to the frozen state, which fixes the conformation (geometric shape) of the macromolecule [26, 27]. The first of these transformations is likely to occur in *block copolymers* A-B, whose structure is an alternation of different blocks consisting each of the same monomers (for example, ...AAABBAABB...). Transformations of the second type, which are a form of vitrification, occur in *disordered heteropolymers* formed by a random sequence of different monomers. In this case even a minor change in the sequence of monomer alteration (or in the parameters of interaction) may cause a major change in the ground state of the heteropolymer. Let us consider each of the above-mentioned transformations.

The thermodynamic state of the block copolymer A-B is defined by the composition parameter $0 \leq f \leq 1$ specifying the proportion of monomers of type A, and the thermodynamic parameter χN , where N is the polymerization index, and χ is the Flory–Huggins parameter which characterizes the difference in the interaction of monomers of different types with respect to the temperature. The first theory of microphase separation was constructed by Flory [35]; however, his macroscopic approximation did not provide for taking into account the mesoscopic nature of phase distribution. Its description can be achieved in the limiting cases of *strong and weak segregation* (in the former case the sharp boundaries between the domains are taken into account, whereas in the latter they are neglected). The self-consistent microscopic theory of microphase separation [34] shows that in the limit of weak segregation at $f = 0.5$ the continuous phase transition from the ‘most ordered’ lamellar mesostructure into the disordered state is realized. As the composition departs from $f = 0.5$, a chain of the first-order transitions is observed: the lamellar mesostructure transforms into the threadlike hexagonal structure, which turns into the body-centered cubic lattice composed of spheroidal precipitates of a different composition; more complicated structures are also observed [26]. It is characteristic that the period of these mesostructures is of the order of the block size and does not depend on temperature.

An important feature of microphase separation is that the fluctuations, owing to the presence of spatially periodic structure, modify considerably the thermodynamic pattern of phase transition [36]. Indeed, in spatially homogeneous systems the fluctuation correction comes from the Bogolyubov singularity \mathbf{k}^{-2} at the origin $\mathbf{k} = 0$ of the wave space. After integration over the volume of the d -dimensional \mathbf{k} -space, this correction assumes the order of k_0^{d-2} , where k_0 is the characteristic wave number. Because of this, fluctuations of the order parameter in homogeneous systems (where

$k_0 \rightarrow 0$) are only important when $d < 2$. The situation is completely different in the presence of spatially periodic structure characterized by the wave vector \mathbf{k}_0 . Here, the singularity $(\mathbf{k} - \mathbf{k}_0)^{-2}$ reveals itself not at one point, but on the surface of the sphere $|\mathbf{k}| = k_0$. This leads to the singular positive addition to the coefficient of the quadratic term in Landau’s expansion, because of which the second-order phase transition becomes a transition of the first order. In block copolymers, this feature considerably modifies the phase diagram, in particular, near the composition $f = 0.5$ there appears a broad ‘window’ where the lamellar phase can directly transfer to the disordered phase [37]. A very peculiar situation is observed with the *disordered block copolymers* which exhibit properties shown both by regular block copolymers and by disordered heteropolymers (see below). The study of such systems [38], based on the transfer matrix method which allows one to take into account the short-range correlations, indicates that the two-phase regions appear in the phase diagram, while the characteristic period begins to depend on the external conditions, which is a feature of disordered systems.

As mentioned above, the disordered heteropolymer is capable of vitrification (freezing), at which the state is realized with a fixed configuration of the chain and a prescribed composition sequence of monomer alternations. The most popular example of vitrification is the protein coagulation which consists in the capability of the macromolecule to find the 3D conformation and the sequence of nucleotides corresponding to the existing external conditions. The unique nature of this phenomenon is demonstrated by *Leveanth’s paradox*, which states that a polymer chain consisting of $N \gg 1$ monomers is capable of arranging itself into the required conformation from the set that includes an exponentially large number of states, $\exp(\alpha N)$, where $\alpha \sim 1$. This problem was encountered for the first time in the study of spin glasses which differ from disordered heteropolymers only in that the quenched disorder in spin glasses results from the quenching of a disordered state, whereas in polymers it is fixed by the composition sequence of monomers, which arises on synthesis of the macromolecule. The analogy between spin glasses and disordered heteropolymers allowed the vitrification temperature of the heteropolymer represented by the ‘many letter sequence’ [39] to be found, and the study of the simultaneous pattern of vitrification and microphase separation that may precede freezing [40] to be conducted. It turns out that the vitrification temperature decreases when the overlapping between different replicas is taken into account [41].

An understanding of the main features of the process of vitrification may be achieved in the context of the simplest method of random energies [28]. This method is based on the assumption that the energy spectrum of a disordered system consists of discrete and continuous components, the latter of which gives the main contribution to the thermodynamic characteristics [29], whereas the corresponding energies are distributed in a practically independent way [42, 43]. To look into the essence of the method we provide for the fact that the number of microstates available for $N \gg 1$ particles amounts to $\mathcal{M} \sim \exp(\alpha N) \rightarrow \infty$, $\alpha \sim 1$. The probability of realization of a microstate with energy E obeys the simplest Gauss distribution

$$P(E) \propto \exp\left(-\frac{E^2}{2N\mathcal{E}^2}\right),$$

where \mathcal{E} is the width of energy spread. The density of states $\mathcal{N}(E) = \mathcal{M}P(E)$ assumes astronomically large values near $E = 0$, and falls off rapidly at $E < 0$. The lower edge of the continuous spectrum E_b is given by the condition $\mathcal{N}(E) \sim 1$, according to which $E_b \approx -\mathcal{E}N$. In this way, the width of the region that gives the definitive contribution to the thermodynamic characteristics is proportional to the number of particles N . On the other hand, the width of the discrete spectrum depends on the energy spread and is proportional to $\sim \mathcal{E}N^{1/2}$, which is negligibly small compared to $E_b \propto N$ in the thermodynamic limit $N \rightarrow \infty$. Precisely this circumstance allows us to neglect the contribution from the discrete states, in spite of the fact that these states determine the state of the glass. In its turn the independence of the energy distribution of microstates E allows us to perform averaging of the free energy under the assumption that

$$\bar{F} \equiv -T \ln \bar{Z} \approx -T \ln \bar{Z}.$$

In other words, the averaging of free energy in the random energy approximation is extended to the statistical sum

$$\bar{Z} = \int_{-\infty}^{\infty} \exp\left(-\frac{E}{T}\right) \mathcal{N}(E) dE \approx \mathcal{M}P(E_s) \exp\left(-\frac{E_s}{T}\right). \quad (1.1)$$

In the second equality here we have considered that the integrand has a maximum at the saddle point $E_s = -(\mathcal{E}^2/T)N$. Obviously, the continuous spectrum gives the main contribution under the condition $E_s \geq E_b$, according to which the freezing temperature $T_f \approx \mathcal{E}$. At $T < T_f$, when $E_s \leq E_b$, the main contribution to the statistical sum comes from the discrete spectrum, and the random energy approximation is no longer valid. However, since in the glassy state all microscopic states except a few are frozen out, the dependence on temperature disappears and the thermodynamic quantities assume the values corresponding to the freezing point T_f .

Of course, this situation is not a consequence of the free energy approximation, but is an attribute of disordered systems. This is associated with the appearance of a hierarchy of thermodynamic variables when ergodicity is violated, caused by the contribution from the discrete spectrum. This hierarchy lies in the separation of the thermodynamic parameters into the microscopic and macroscopic magnitudes: the former correspond to the continuous spectrum whose energy distribution E depends on the thermal disorder (temperature), whereas the latter relate to the discrete component characterized by quenched disorder. As a result, the microscopic quantities are determined by the temperature, and the macroscopic by the intensity of quenched disorder [44].

As follows from the arguments developed above, the main problem in the treatment of disordered systems is associated with averaging of the logarithmic function. To overcome this difficulty, Edwards and Anderson [14] proposed using the limit

$$\ln Z = \lim_{n \rightarrow 0} \frac{Z^n - 1}{n}. \quad (1.2)$$

The presence of the exponential function Z^n indicates that in place of one thermodynamic system with the statistical sum Z one should take the number $n \rightarrow 0$ of systems (replicas) identical to the original one. Recently, the replic method was further developed in the theory of nonadditive systems [6]. It

turned out that the behavior of such systems can only be understood if the nonadditivity parameter n is nonzero. Then the space of states assumes a fractal character, which leads to its separation into isolated clusters corresponding to different replicas.

The results obtained with the replic method were reproduced using the Langevin equation for the ‘soft’ spin model [45]. This exercise resulted in a self-consistent set of dynamic equations in the response function and structural factor, ‘extended’ by adding the nonergodicity and memory parameters.

Like for all systems with quenched disorder, the description of disordered heteropolymers calls for averaging over the appropriate distribution (composition disorder). As indicated above, harnessing the random energy method assumes that the microstates are distributed independently, which is actually not the case. On the other hand, the replic method is based on a mathematical trick and requires cumbersome calculations, the physical content of which is not always clear. The use of dynamic equations is not very promising, because they are much complicated by the presence of the covalent bond that leads to the formation of the polymer chain [25]. All this points to the expedience of the construction of a microscopic theory of disordered heteropolymers, which gives a consistent treatment to the effects of memory and nonergodicity. We propose to use the theory of supersymmetric field as the scheme appropriate for resolving this problem [46–48]. It leads to a set of equations that self-consistently describe the behavior of a nonequilibrium thermodynamic system possessing memory and nonergodicity [49].

Being a version of the field-theoretical scheme, our approach is based on the generating functional method proposed by Martin, Siggia and Rose [50] (see also Refs [51, 52]). The formal base for the introduction of the supersymmetric field is the nilpotent quantity representing the square root of 0. In this sense, the superfield is similar to the complex field in which the imaginary unit equal to square root of -1 is used in place of the anticommuting nilpotent quantity (the Grassmann variable). By definition, the supersymmetric field unites the commuting boson components and the anticommuting fermion components into a unified mathematical construction represented by a vector in the supersymmetric space. Such fields were first introduced in the quantum field theory [53–55], and later applied to the analysis of stochastic systems [56, 57]. They served as a basis for the self-consistent microscopic theory of spin glasses [44], later extended to the description of nonequilibrium thermodynamic systems [58]. Within the framework of the Sherrington–Kirkpatrick model it was demonstrated that the supersymmetric scheme is identical to the replica approach [59]. The supersymmetric field was applied to polymers in paper [60]; however, the proposed methods have not been developed any further. Neither is it possible to use the supersymmetric scheme developed in the theory of spin glasses, because the equation of motion of the polymer chain [25] becomes so complicated owing to the presence of the covalent bond that is can no longer be used as the basis of the generating functional method.

Despite the considerable progress in the supersymmetric theory of nonequilibrium thermodynamic systems, there are still a number of outstanding fundamental issues remained unsettled. First of all, it turns out that the representation of the supersymmetric field is not unique — both in the sense of

the physical interpretation of its components and the number of the latter. Consequently, the expansion of the supersymmetric correlator in terms of the components is also not unique, which makes it necessary to select the optimal basis whose components would yield the structural factor and the Green function. The ultimate task is to develop the simplest supersymmetric scheme that would describe in a self-consistent way the effects of memory and nonergodicity depending on the intensities of thermal and quenched disorders. This problem is solved in Section 2, and the especially formal constructions are moved out to the appendices.

In Section 3, the Edwards Hamiltonian is used for expressing the free energy of the heterophase polymer, which acts as the effective Lagrangian in the supersymmetric field theory. This expression allows one to take into account both the overlapping of replicas and the fluctuation effects.

As indicated above, the main problem in the construction of the field-theoretical scheme of heterophase polymer consists in that the original equation of motion is so complicated that it cannot be used for finding the generating functional. Because of this, Section 4 starts with construction of the effective equation of motion of disordered heteropolymer that reflects the stochastic alternation of monomers of different kinds as we move along the polymer chain. This allows the correlation technique developed in Section 2 to be used for a self-consistent description of the memory and nonergodicity effects of a disordered heteropolymer, depending on its composition, thermal and quenched disorders. The results are summarized in Section 5.

2. Supersymmetric representation of a nonequilibrium stochastic system

As noted in the previous section, the introduction of the superfield — a combination of the conventional and Grassmann components — is an extension of the basis as natural as the transition from real to complex fields. Now we shall show that the supersymmetric approach allows a complete description of an arbitrary (possibly nonequilibrium) stochastic system with quenched disorder [49, 58]. This is accomplished by expanding the correlator of the superfield with respect to the closed basis whose coefficients reduce to the observable quantities: the structural factor $S(\omega)$ and retarded/advanced Green functions $G_{\pm}(\omega)$, where ω is the frequency. The inclusion of memory and nonergodicity gives added terms $S(0) \propto q$, $G_{\pm}(0) \equiv \Delta$, which correspond to the hydrodynamic limit $\omega = 0$. As a result, the supersymmetric self-consistent scheme permits one to obtain the equations in parameters of memory q and nonergodicity Δ .

In the construction of the supersymmetric theory it is important to remember that the superfield, like any gauge field, may turn out to be reducible (like the four-component electromagnetic field can break down into the vector and scalar components). Indeed, the condition of gauge invariance leads to decomposition of the superfield into chiral components, each one-half the dimension of the original superfield [52]. For our case of a disordered heteropolymer, we shall demonstrate that in the limit of weak segregation the condition of entropy conservation, imposed on the original four-component superfield, leads to the separation of the irreducible component in the form of a two-component (*dual*) Bose field. Then the first component has the meaning of the order parameter, and the second component refers to the conjugate field or the amplitude of its fluctuations.

In the calculation of observable quantities, the judicious selection of the basis used for expanding the supercorrelator is important. For example, a three-component basis was used in Ref. [44], whose components G_0 , G_1 , S give the advanced $G_+ \equiv G_0 + G_1$ and the retarded $G_- \equiv G_0 - G_1$ Green functions, as well as the structural factor S . The addition of the fourth component in work [61] was necessary because the supersymmetric field here contains the field itself rather than the amplitude of fluctuations of the conjugate field whose static correlator reduces to zero. Since the correlator of the field is $S_- \neq 0$, the basis for expansion of the supercorrelator must contain the quantities S , G_+ , G_- , S_- , and must therefore have four components. Further extension of the basis (to six components) is needed when the reactive regime is taken into account in addition to the dissipative regime [58]. Among the considerations then are the effects of self-organization, which lead to violation of the condition of entropy conservation [62]. Here, however, we shall not touch upon such synergetic effects, confining ourselves to homogeneous thermodynamic systems, for which the correlators of the Grassmann components of the superfield reduce to the Green functions G_{\pm} . Inasmuch as the correlator of fluctuations included in the superfield is $S_- \equiv 0$, and the parameters of nonergodicity and memory are included in G_{\pm} , S , it is clear that a basis of dimension 3 is sufficient for the description of a nonequilibrium stochastic system. Precisely this case was considered in Ref. [44]; however, the selected basis is not optimal because it gives not the observed Green functions G_{\pm} , but their components $G_{0,1} = (G_+ \pm G_-)/2$.

This section is devoted to the construction of a supersymmetric scheme that represents the effects of memory and nonergodicity for a nonequilibrium stochastic system in the most rational way [49]. In Section 2.1 we present the field-theoretical scheme based on the method of generating functionals. Using the Langevin equation with white noise, we find the Lagrangian of the system and derive the equations of motion, describing the kinetics of phase transitions. In Section 2.2 we present the simplest superfield scheme based on the two-component dual fields: in Section 2.2.1, we consider the case when the second component is the amplitude of fluctuations, and the conjugate field in Section 2.2.2. Section 2.2.3 is concerned with the analysis of the linkage between these representations, and we express the operators of transitions between them. In Section 2.3 we present the scheme that allows the original four-component superfields to be reduced to the two-component form which, however, does not coincide with the chiral superfield. In Section 2.4 the supercorrelator is expanded in terms of the basis operators, and the coefficients of expansion reduce to the observables G_{\pm} , S . We demonstrate that the reduction of the four-component superfield to the two-component field corresponds to the reduction in the dimension of the superbasis used for the expansion of the supercorrelator. This becomes possible thanks to the adoption of the Ward identity which leads to the equality between correlators of Grassmann fields and the corresponding Green functions. In Section 2.5 we present the supersymmetric perturbation theory used for expressing the components Σ_{\pm} , Σ of the expansion of the self-energy superfunction. Their definition is based on the ϕ^4 and ϕ^3 models of perturbation theory with respect to anharmonism (Sections 2.5.1 and 2.5.2, respectively). However, unlike work [44], in the definition of the Fourier transform of the component $\Sigma_-(\omega)$ containing convolutions we proceed not from the use of the bare

functions but the fluctuation-dissipative theorem which allows the exact expression for $\Sigma_-(\omega)$ to be found. In Section 2.6, we first (Section 2.6.1) present the self-consistent scheme allowing one to construct the effective Lagrangian which takes into account both the self-action and the effects of direct and effective interactions (the latter being the result of quenched disorder). In Section 2.6.2, we use this Lagrangian to obtain the supersymmetric Dyson equation. Section 2.7 deals with the equations in the parameters of nonergodicity and memory; they are analyzed in the subsequent Section 2.8. We find here the dependences on the temperature and the intensity of quenched disorder of microscopic and macroscopic susceptibilities and the corresponding memory and nonergodicity parameters. Finally, Section 2.9 deals with the analysis of behavior of the system occurring in a nonstationary state.

2.1 Generating functional

Let us represent the behavior of a stochastic system by the amplitude of the hydrodynamic mode as a space-time function $x(\mathbf{r}, t)$, whose mean value reduces to the order parameter [33]. The description of this function is based on the Langevin equation [63]

$$\dot{x}(\mathbf{r}, t) - D \nabla^2 x = -\gamma \frac{\partial V}{\partial x} + \zeta(\mathbf{r}, t). \quad (2.1)$$

Here the dot overhead denotes the time derivative $\nabla \equiv \partial/\partial \mathbf{r}$, D is the diffusion coefficient, γ the kinetic coefficient, $V(x)$ the effective potential (Landau's free energy), and $\zeta(\mathbf{r}, t)$ the stochastic addition defined by the conditions of white noise:

$$\langle \zeta(\mathbf{r}, t) \rangle_0 = 0, \quad \langle \zeta(\mathbf{r}, t) \zeta(\mathbf{0}, 0) \rangle_0 = \gamma T \delta(\mathbf{r}) \delta(t), \quad (2.2)$$

where the angle brackets $\langle \dots \rangle_0$ denote averaging with respect to the Gaussian distribution of the quantity ζ , and T is the thermostat temperature that determines the noise intensity. The last equality in Eqn (2.2) is often written using a normalization that is twice as large as the one adopted here. This leads to the standard forms of the Onsager relation and the Fokker–Planck equation, in which the factor 1/2 does not appear in front of the diffusion term, but the time dependence $(dx)^2 = D dt$ features the coefficient 2, and under the exponential of the distribution $P_0\{\zeta\}$ in the stochastic variable ζ appears the numerical factor 1/2 (see Ref. [64]). Since our subsequent calculations are based on the assumption of a Gaussian distribution $P_0\{\zeta\}$, we prefer to use a normalization (2.2) that leads to the Gaussian (2.5).

It is also convenient to use further the units $t_s \equiv (\gamma T)^2/D^3$, $r_s \equiv \gamma T/D$, $V_s \equiv D^3/(\gamma^3 T^2)$, $\zeta_s \equiv D^3/(\gamma T)^2$ for the time t , coordinate \mathbf{r} , effective potential V and stochastic variable ζ , respectively (assuming that the amplitude x of the hydrodynamic mode has already been normalized to x_s). Then the equation of motion (2.1) takes on the canonical form

$$\dot{x}(\mathbf{r}, t) = -\frac{\delta V}{\delta x} + \zeta(\mathbf{r}, t), \quad (2.3)$$

where we have used the compact notation for the variational derivative

$$\frac{\delta V}{\delta x} \equiv \frac{\delta V\{x(\mathbf{r}, t)\}}{\delta x(\mathbf{r}, t)} = \frac{\partial V(x)}{\partial x} - \nabla^2 x, \quad V\{x\} \equiv \int \left[V(x) + \frac{1}{2} (\nabla x)^2 \right] d\mathbf{r}. \quad (2.4)$$

In equation (2.2), the coefficient γT disappears, and the distribution in variable ζ assumes the standard Gaussian form

$$P_0\{\zeta\} \propto \exp\left(-\frac{1}{2} \int \zeta^2(\mathbf{r}, t) d\mathbf{r} dt\right). \quad (2.5)$$

Our construction of the field-theoretical scheme is based on the generating functional method [51]

$$Z\{u(\mathbf{r}, t)\} = \int Z\{x\} \exp\left(\int u x d\mathbf{r} dt\right) D x, \quad (2.6)$$

$$Z\{x(\mathbf{r}, t)\} \equiv \left\langle \prod_{(\mathbf{r}, t)} \delta\left\{\dot{x} + \frac{\delta V}{\delta x} - \zeta\right\} \det\left[\frac{\delta \zeta}{\delta x}\right] \right\rangle_0, \quad (2.7)$$

whose variation with respect to the test field $u(\mathbf{r}, t)$ yields the correlators of the observables [see Eqn (2.84)]. Obviously, $Z\{u\}$ is the functional Laplace transform for the function $Z(x)$; the δ function in Eqn (2.7) takes into account the form of equation (2.3), and the determinant describes the transition from the continual integration over ζ to x .

2.2 The use of dual fields

For further development of the field-theoretical scheme we need to establish the type of linkage between the stochastic variables ζ and x . As shown in Section 2.3, for thermodynamic systems in which the state of the thermostat does not depend on x , this linkage is characterized by the constant value of the Jacobian $\det|\delta \zeta/\delta x| = 1$ in expression (2.7). As will be shown below, the thermodynamic system in this case is represented by the two-component commuting fields that contain the nilpotent quantity $\vartheta \equiv \sqrt{0}$. Such fields are aptly referred to as dual.

2.2.1 Amplitude of fluctuations as a component of a dual field.

We start off with the functional representation

$$\delta\{x(\mathbf{r}, t)\} = \int_{-i\infty}^{i\infty} \exp\left(-\int p x d\mathbf{r} dt\right) D p, \quad (2.8)$$

where we introduced the field $p(\mathbf{r}, t)$ whose physical meaning will be identified later. After averaging with respect to distribution (2.5), the functional (2.7) reduces to the standard form

$$Z\{x(\mathbf{r}, t)\} = \int \exp[-S\{x(\mathbf{r}, t), p(\mathbf{r}, t)\}] D p. \quad (2.9)$$

Here, the action $S = \int L d\mathbf{r} dt$ measured in units of $S_s = \gamma^2 (T/D)^3$ is defined by the Lagrangian of the Euclidean field theory:

$$L(x, p) = \left(p \dot{x} - \frac{1}{2} p^2\right) + p \frac{\delta V}{\delta x}. \quad (2.10)$$

To bring the Lagrangian (2.10) to the canonical form, we introduce the dual field

$$\phi_p = x + \vartheta p \quad (2.11)$$

with the Bose components x, p , and the nilpotent quantity ϑ , as defined by the equations

$$\vartheta \vartheta' - \vartheta' \vartheta = 0, \quad \int d\vartheta = 0, \quad \int \vartheta d\vartheta = 1. \quad (2.12)$$

As shown in Appendix A, in the representation (2.11) the expression in the first parentheses of the Lagrangian (2.10) takes on the form

$$\kappa = \frac{1}{2} \int \phi D\phi d\vartheta \quad (2.13)$$

inhering in the kinetic energy in Dirac's field-theoretical scheme [51]. The Hermitian operator D is given by the expression

$$D_p = -\frac{\partial}{\partial \vartheta} + \left(1 - 2\vartheta \frac{\partial}{\partial \vartheta}\right) \frac{\partial}{\partial t} \quad (2.14)$$

and satisfies conditions (6.6). On the other hand, the conditions of nilpotency permit one to write the last term in equality (2.10) in the standard form (see Appendix A):

$$\pi = \int V(\phi) d\vartheta. \quad (2.15)$$

As a result, the Lagrangian (2.10) takes on the canonical form¹

$$L \equiv \kappa + \pi = \int \lambda d\vartheta, \quad \lambda(\phi) \equiv \frac{1}{2} \phi D\phi + V(\phi). \quad (2.16)$$

As shown in Appendix A, expressions (2.10), (2.16) are invariant with respect to the transform $\exp(\varepsilon D)$, set by the generator (2.14). The parameter $\varepsilon \rightarrow 0$ is then purely imaginary, and the fields $x(\mathbf{r}, t)$, $p(\mathbf{r}, t)$ are complex.

When an infinitesimal increment $\delta\phi$ is added to the field ϕ , the action

$$s\{\phi(\zeta)\} = \int \lambda(\phi(\zeta)) d\zeta, \quad \zeta \equiv \{\mathbf{r}, t, \vartheta\}, \quad (2.17)$$

acquires the addition $\delta s = 0$, if Euler's equation is valid:

$$D \frac{\delta \lambda}{\delta(D\phi)} + \frac{\delta \lambda}{\delta \phi} = 0. \quad (2.18)$$

Substituting here the expression (2.16), we arrive at the equation of motion

$$D\phi + \frac{\delta V}{\delta \phi} = 0 \quad (2.19)$$

which defines the most probable value

$$\phi_p^{(\max)} = \eta + \vartheta\phi, \quad \eta \equiv x^{(\max)}, \quad \phi \equiv p^{(\max)}, \quad (2.20)$$

of the dual field (2.11). Taking the projections of Eqn (2.19) onto the real and the nilpotent axes, we get the set of equations

$$\dot{\eta} = -\frac{\delta V}{\delta \eta} + \phi, \quad (2.21)$$

$$\dot{\phi} = \frac{\delta^2 V}{\delta \eta^2} \phi \quad (2.22)$$

that describe the kinetics of change of the most probable values $x^{(\max)} \equiv \eta$, $p^{(\max)} \equiv \phi$. The comparison of equation (2.21) with the Langevin equation (2.3) indicates that the ghost field $p(\mathbf{r}, t)$ introduced in the integral representation (2.8) reduces to the amplitude of fluctuations $\zeta(\mathbf{r}, t)$ of the force conjugate to the amplitude of the hydrodynamic mode, and the quantity $\phi \equiv p^{(\max)} \equiv \zeta^{(\max)}$ gives its most probable value. Although the latter may be different from the mean value, we shall call the quantity $\eta \equiv x^{(\max)}$ the *order parameter*.

Equations (2.21), (2.22) corresponding to the minimum of the Lagrangian (2.10) determine the most probable realization $P\{\eta(\mathbf{r}, t), \phi(\mathbf{r}, t)\}$ of the distribution function

$$P\{x(\mathbf{r}, t), p(\mathbf{r}, t)\} = Z^{-1} \exp\left(-\int L(x, p) d\mathbf{r} dt\right) \quad (2.23)$$

of the original fluctuating fields. Here the statistical sum $Z \equiv Z\{u=0\}$ reduces to the generating functional $Z\{u\}$ set by equality (2.6). Obviously, the distribution function $P\{\eta(\mathbf{r}, t), \phi(\mathbf{r}, t)\}$ of the most probable fields $\eta \equiv x^{(\max)}$, $\phi \equiv p^{(\max)}$ answers to the classical approximation of the quantum field theory, which corresponds to the probability density (2.23) (see Ref. [51]).

2.2.2 Conjugate field as a component of a dual field. Let us demonstrate that expression (2.11) is not the only possible dual field that allows the construction of the self-consistent field-theoretical scheme. With this purpose we introduce the field $f(\mathbf{r}, t)$, as defined by the relation

$$\dot{x} = f + p. \quad (2.24)$$

Then the Lagrangian (2.10) becomes

$$L(x, f) = \frac{1}{2} (\dot{x}^2 - f^2) - \frac{\delta V}{\delta x} f + \frac{\delta V}{\delta x} \dot{x}. \quad (2.25)$$

The last term can be dropped out because it is the total derivative $dV\{x\}/dt$ which corresponds to the equilibrium statistical sum

$$Z_0 = \int \exp\left(-\frac{\Delta V\{\eta_i, \eta_f\}}{T}\right) D\eta_i D\eta_f, \quad \Delta V\{\eta_i, \eta_f\} \equiv V\{\eta_i\} - V\{\eta_f\} > 0, \quad (2.26)$$

which does not depend on the intermediate states. Here we returned to the dimensional potential V , where $\eta_i(\mathbf{r}) \equiv x(\mathbf{r}, t_i)$, $\eta_f(\mathbf{r}) \equiv x(\mathbf{r}, t_f)$ are the initial and the final fields of the order parameter, determined by the appropriate distributions of the amplitude of the hydrodynamic mode. Substituting the Lagrangian (2.25) into the Euler equation (2.18), we get the equations of motion

$$\ddot{\eta} = -\frac{\delta^2 V}{\delta^2 \eta} f, \quad (2.27)$$

$$f = -\frac{\delta V}{\delta \eta}, \quad (2.28)$$

which are equivalent to the set (2.21), (2.22). Indeed, if we differentiate equations (2.21) with respect to time, using equality (2.22) and the relation

$$\dot{\eta} = f + \phi \quad (2.29)$$

¹ Hereinafter we drop the subscripts (in this expression p) as long as the resulting expressions do not depend on the selection of field components.

that follows from Eqn (2.24), we immediately arrive at Eqn (2.27). As far as equation (2.28) is concerned, it reduces to the definition of the force $f(\mathbf{r})$ conjugate to the order parameter $\eta(\mathbf{r}, t)$. Since the fluctuations do not affect the macroscopic potential $V(\mathbf{r})$, their inclusion does not change equation (2.28), and therefore the conjugate force f which does not depend explicitly on the time t . It is this circumstance that ensures the similarity of equations (2.24) and (2.29) for random and the most probable fields.

Following definition (2.11), we introduce the dual field [61]

$$\phi_f = x - \vartheta f \quad (2.30)$$

whose Bose components are the amplitude x of the hydrodynamic mode and the conjugate force f taken with the opposite sign. According to Appendix A, the replacement of the second component p in Eqn (2.11) by $-f$ in definition (2.30) retains the dual form of the Lagrangian (2.16) and conditions (6.6). However, the generator of the corresponding symmetry group takes on the form

$$D_f = -\left(\frac{\partial}{\partial \vartheta} + \vartheta \frac{\partial^2}{\partial t^2}\right) \quad (2.31)$$

which, differently from relation (2.14), involves the time derivative of the second order rather than of the first.

2.2.3 Linkage between different dual representations. Let us prove the similarity of the field-theoretical schemes based on the fields (2.11) and (2.30). With this purpose we introduce the transformation operators $\tau_{\pm} = \exp(\pm \vartheta \partial_t)$, $\partial_t \equiv \partial/\partial t$ whose action on the fields ϕ_p , ϕ_f is expressed by the following relations

$$\tau_{\pm} \phi_{\mp p}(t) = \phi_{\mp f}(t), \quad \tau_{\pm} \phi_{\pm f}(t) = \phi_{\pm p}(t). \quad (2.32)$$

In this way, the operators τ_{\pm} transform the dual representations (2.11), (2.30) one into the other if we take the opposite signs for the operator τ_{\pm} and field $\phi_{\mp p}$, and the same signs for τ_{\pm} and $\phi_{\pm f}$. On the other hand, performing an expansion into a power series of ϑ with due account for Eqns (2.12), (2.24), we get

$$\phi_{\mp p}(t \pm \vartheta) = \phi_{\mp f}(t), \quad \phi_{\pm f}(t \pm \vartheta) = \phi_{\pm p}(t). \quad (2.33)$$

Comparing expressions (2.32), (2.33) we see that the operators τ_{\pm} shift the physical time t by the magnitude of the nilpotent coordinate $\pm \vartheta$ if the amplitude p of fluctuations has the opposite sign, and the sign of force coincides with the sign in the subscript of operator τ_{\pm} :

$$\tau_{\pm} \phi_{\mp p}(t) = \phi_{\mp p}(t \pm \vartheta), \quad \tau_{\pm} \phi_{\pm f}(t) = \phi_{\pm f}(t \pm \vartheta). \quad (2.34)$$

These equalities can also be expressed in the framework of the matrix representation as defined by expressions (6.7), (6.9) and (6.10) in Appendix A. Transformations of dual fields, $\tau_{+} \phi_f = \phi_p$, $\tau_{-} \phi_p = \phi_f$, correspond to the relations between generators (2.14), (2.31):

$$D_f = \tau_{-} D_p \tau_{+}, \quad D_p = \tau_{+} D_f \tau_{-}. \quad (2.35)$$

It is easy to verify that the condition $\dot{f} \equiv 0$ leads to the invariance of the kernel λ in the definition of Lagrangian (2.16).

2.3 Reduction of a supersymmetric field to the dual form

The approach developed in the previous section is based on the simplest assumption that the Jacobian in equality (2.7) is $\det |\delta \zeta / \delta x| = 1$. In the general case, for an arbitrary matrix $|A|$ we have

$$\det |A| = \int \exp(\bar{\psi} A \psi) d^2 \psi, \quad d^2 \psi = d\psi d\bar{\psi}, \quad (2.36)$$

where $\psi(\mathbf{r}, t)$, $\bar{\psi}(\mathbf{r}, t)$ are the Grassmann conjugate anti-commuting fields subject to the conditions [cf. Eqn (2.12)]

$$\begin{aligned} \bar{\psi} \psi + \psi \bar{\psi} &= 0, & \int d\psi &= 0, & \int \psi d\psi &= 1, \\ \int d\bar{\psi} &= 0, & \int \bar{\psi} d\bar{\psi} &= 1. \end{aligned} \quad (2.37)$$

Physically speaking, the appearance of the new degrees of freedom ψ , $\bar{\psi}$ is conditioned by the inclusion of feedback that makes the state of the thermostat dependent on the order parameter. Such a situation is inherent in self-organizing systems [62]. As a result, the Lagrangian (2.10) supplemented by the Grassmann fields ψ , $\bar{\psi}$ becomes

$$\mathcal{L}(x, p, \psi, \bar{\psi}) = \left(p \dot{x} - \frac{p^2}{2} + \frac{\delta V}{\delta x} p \right) - \bar{\psi} \left(\frac{\partial}{\partial t} + \frac{\delta^2 V}{\delta x^2} \right) \psi. \quad (2.38)$$

Introducing the four-component superfield

$$\Phi_p = x + \bar{\theta} \psi + \bar{\psi} \theta + \bar{\theta} p, \quad (2.39)$$

similarly to the previous section we get the supersymmetric Lagrangian

$$\begin{aligned} \mathcal{L} &= \int \Lambda d^2 \theta, \quad d^2 \theta \equiv d\theta d\bar{\theta}, \\ \Lambda(\Phi_p) &\equiv \frac{1}{2} (\bar{\mathcal{D}}_p \Phi_p) (\mathcal{D}_p \Phi_p) + V(\Phi_p), \end{aligned} \quad (2.40)$$

where θ , $\bar{\theta}$ are the Grassmann conjugate coordinates defined by expressions similar to Eqns (2.37):

$$\begin{aligned} \bar{\theta} \theta + \theta \bar{\theta} &= 0, & \int d\theta &= 0, & \int \theta d\theta &= 1, \\ \int d\bar{\theta} &= 0, & \int \bar{\theta} d\bar{\theta} &= 1. \end{aligned} \quad (2.41)$$

Later on we shall establish a link between the Grassmann coordinates θ , $\bar{\theta}$ and the earlier introduced nilpotent quantity ϑ defined by conditions (2.12). As compared with equality (2.16), where the kernel λ had the first power of the generator (2.14), the Lagrangian (2.38) involves a pair of operators

$$\mathcal{D}_p = \frac{\partial}{\partial \theta} - 2\theta \frac{\partial}{\partial t}, \quad \bar{\mathcal{D}}_p = \frac{\partial}{\partial \bar{\theta}} \quad (2.42)$$

that do not satisfy the conditions of Grassmann conjugation. The corresponding supersymmetric Euler equation is

$$-\frac{1}{2} [\bar{\mathcal{D}}, \mathcal{D}] \Phi + \frac{\delta V}{\delta \Phi} = 0, \quad (2.43)$$

where the brackets denote the commutator. Taking the projections of Eqn (2.43) onto the axes 1, $\bar{\theta}$, θ , and $\bar{\theta}\theta$, we

get the equations of motion

$$\dot{\eta} - \nabla^2 \eta = -\frac{\partial V}{\partial \eta} + \varphi, \quad (2.44)$$

$$\dot{\varphi} + \nabla^2 \varphi = \frac{\partial^2 V}{\partial \eta^2} \varphi - \frac{\partial^3 V}{\partial \eta^3} \bar{\psi} \psi, \quad (2.45)$$

$$\dot{\psi} - \nabla^2 \psi = -\frac{\partial^2 V}{\partial \eta^2} \psi, \quad (2.46)$$

$$-\dot{\bar{\psi}} - \nabla^2 \bar{\psi} = -\frac{\partial^2 V}{\partial \eta^2} \bar{\psi} \quad (2.47)$$

that define the most probable realizations of the fields $\eta \equiv x^{(\max)}$, $\varphi \equiv p^{(\max)}$, $\psi^{(\max)}$, and $\bar{\psi}^{(\max)}$ (in the last two we dropped out the superscripts ‘max’ for brevity). At $\psi = \bar{\psi} = 0$, these equations reduce to the corresponding equalities (2.21), (2.22) for dual fields. Combining the pair of equations (2.46), (2.47), we get the conservation law $\dot{S} + \nabla \mathbf{j} = 0$ for the quantities

$$S = \bar{\psi} \psi, \quad \mathbf{j} = (\nabla \bar{\psi}) \psi - \bar{\psi} (\nabla \psi). \quad (2.48)$$

In the case of inhomogeneous thermodynamic systems, the quantity S acts as the density of the interphase boundaries, and \mathbf{j} is the corresponding flux [58]. In this way, in the theory of polymers the four-component field corresponds to the limit of strong segregation, used in Ref. [65]. For self-organizing systems, the quantity S is the entropy, and \mathbf{j} is the probability flux [49]. For thermodynamic systems, where the entropy is conserved, the Grassmann fields $\psi(\mathbf{r}, t)$, $\bar{\psi}(\mathbf{r}, t) = \text{const}$ can be dropped out, and the four-component supersymmetric field (2.39) reduces to the two-component dual form (2.11).

To accomplish this reduction, we write down the kinetic energy of the super-Lagrangian (2.40) in the form

$$-\frac{1}{4} \Phi_\varphi [\bar{\mathcal{D}}_\varphi, \mathcal{D}_\varphi] \Phi_\varphi,$$

where, accurately to the replacement $p \rightarrow \varphi$, the quantities Φ_φ , \mathcal{D}_φ are defined by the equalities (2.39), (2.42), and the commutator assumes the form

$$-\frac{1}{2} [\bar{\mathcal{D}}_\varphi, \mathcal{D}_\varphi] = -\frac{\partial^2}{\partial \theta \partial \bar{\theta}} + \left(1 - 2\theta \frac{\partial}{\partial \theta}\right) \frac{\partial}{\partial t}. \quad (2.49)$$

Obviously, this expression reduces to the dual form (2.14) if we set $\vartheta \equiv \bar{\theta}\theta$. Then, the anticommuting Grassmann variables θ , $\bar{\theta}$ transform into the self-conjugate commuting variable ϑ .

Similarly to Sections 2.2.1, 2.2.2, we may show that the use of linkage (2.24) allows one to go from the amplitude p of fluctuations to the conjugate force f . Then, the first parenthesis in the Lagrangian (2.38) takes on the form (2.25), and in place of the system (2.44)–(2.47) we get the equation [cf. Eqn (2.27)]

$$\ddot{\eta} = -\frac{\delta^2 V}{\delta \eta^2} f - \frac{\delta^3 V}{\delta \eta^3} \bar{\psi} \psi \quad (2.50)$$

supplemented by definition (2.28) and equations (2.46), (2.47) for the Grassmann fields $\psi(\mathbf{r}, t)$, $\bar{\psi}(\mathbf{r}, t)$. By analogy with the case of dual fields considered above, the equation of motion (2.50) can be found by time-differentiation of equality (2.44), using formulas (2.29), (2.45). The corresponding Lagrangian $\mathcal{L}(x, f, \psi, \bar{\psi})$ assumes the following supersymmetric form [cf.

Eqn (2.40)]

$$\mathcal{L} = \int \Lambda d^2 \theta, \quad \Lambda(\Phi_f) \equiv -\frac{1}{2} \Phi_f \bar{\mathcal{D}}_f \mathcal{D}_f \Phi_f + V(\Phi_f), \quad (2.51)$$

if we introduce the superfield [cf. definition (2.30)]

$$\Phi_f = x + \bar{\theta} \psi + \bar{\psi} \theta - \bar{\theta} \theta f; \quad (2.52)$$

$$\Phi_f = \Phi_p - \bar{\theta} \theta \dot{\Phi}_f = T_- \Phi_p,$$

$$T_\pm \equiv \exp(\pm \bar{\theta} \theta \partial_t), \quad \partial_t \equiv \frac{\partial}{\partial t}.$$

The Grassmann conjugate operators \mathcal{D}_f , $\bar{\mathcal{D}}_f$ appear as follows [cf. Eqn (2.42)]

$$\mathcal{D}_f = \frac{\partial}{\partial \theta} - \theta \frac{\partial}{\partial t}, \quad \bar{\mathcal{D}}_f = \frac{\partial}{\partial \bar{\theta}} - \bar{\theta} \frac{\partial}{\partial t}. \quad (2.53)$$

It is easy to demonstrate that the superfields (2.39), (2.52) are transformed into each other similarly to equalities (2.32)–(2.34) if we replace the transformation operators $\tau_\pm = \exp(\pm \vartheta \partial_t)$ by $T_\pm \equiv \exp(\pm \bar{\theta} \theta \partial_t)$. On the other hand, by analogy with Eqn (2.35), the pairs of conjugate superoperators (2.42), (2.53) are linked by the transformation

$$\mathcal{D}_f = T_- \mathcal{D}_\varphi T_+, \quad \bar{\mathcal{D}}_f = T_- \bar{\mathcal{D}}_\varphi T_+. \quad (2.54)$$

According to Eqn (2.53), for the product of operators in the kernel of supersymmetric Lagrangian (2.51) we have [cf. Eqn (2.49)]

$$-\bar{\mathcal{D}}_f \mathcal{D}_f = -\left(\frac{\partial}{\partial \theta} \frac{\partial}{\partial \bar{\theta}} + \bar{\theta} \theta \frac{\partial^2}{\partial t^2}\right) + \left(\bar{\theta} \frac{\partial}{\partial \bar{\theta}} - \theta \frac{\partial}{\partial \theta}\right) \frac{\partial}{\partial t}. \quad (2.55)$$

This expression reduces to operator (2.31) if we set $\bar{\theta}\theta \equiv \vartheta$ and note that $\bar{\theta}(\partial/\partial \bar{\theta}) = \theta(\partial/\partial \theta)$.

In this way, the four-component Grassmann fields (2.39), (2.52) reduce to the two-component forms (2.11), (2.30). Accordingly, the supersymmetric generators (2.42), (2.53) go over into expressions (2.14), (2.31).

This reduction of superfields can be derived from the calibration conditions

$$\mathcal{D}\Phi = 0, \quad \bar{\mathcal{D}}\Phi = 0. \quad (2.56)$$

Indeed, in accordance with definitions (2.39), (2.42), (2.52), (2.53), the equalities (2.56) produce the linkage

$$\bar{\theta} \psi + \bar{\psi} \theta - 2\bar{\theta} \theta f = 0 \quad (2.57)$$

which, given that $\vartheta \equiv \bar{\theta}\theta$, reduces the supersymmetric field (2.52) to the form (2.30) with the opposite sign in front of f .

In spite of their having an equal number of components, the physical meaning of the above-introduced dual fields (2.11), (2.30) is different from that of the Grassmann conjugate pair of chiral fields (6.26), which are the result of the supersymmetric gauge invariance (see Appendix B). The main distinction is that the dual fields ϕ_p , ϕ_f consist of the pairs of Bose components x , p and x , f , whereas the chiral superfields ϕ_+ , ϕ_- are combinations of the Bose component x and the Fermi components ψ , $\bar{\psi}$. This distinction comes from the fact that when the chiral superfields are singled out, the condition of supersymmetric gauge invariance (6.24) is imposed not on the original supersymmetric field Φ satisfying equalities (2.56) but rather on the components Φ_\pm that are

obtained from Φ by the action of operators $T_{\pm} = \exp(\pm \bar{\theta} \partial_t)$ [see Eqn (6.18)].

To visualize the difference between the dual fields (2.11), (2.30) and the chiral field (6.26), let us consider the supersymmetric field (2.52) as a vector in the four-dimensional space with axes $\theta^0 = \bar{\theta}^0 \equiv 1$, $\bar{\theta}$, θ , $\bar{\theta}\theta \equiv \vartheta$. Then calibration (2.56) reduces the field (2.52) to the vector (2.30) located in the plane running along the axes 1, ϑ . Accordingly, the calibration (6.24) leads to the partition of the total supersymmetric space into two orthogonal subspaces, the first of which is formed by the axes 1, θ and contains the vector ϕ_- , whereas the second is formed by the axes 1, $\bar{\theta}$ and contains the vector ϕ_+ . Since these subspaces are Grassmann conjugate ($\phi_- = \phi_+$), it will suffice to consider only one of them, using either vector ϕ_- or ϕ_+ (see Appendix B). Such a program was carried out in Ref. [66], where the earlier used dual field (2.30) was obtained by projecting the chiral vectors ϕ_{\pm} onto the plane formed by the axes 1, ϑ . Hence it follows that our approach based on the adoption of dual fields (2.11), (2.30) is equivalent to the theory developed in Ref. [66]. The supersymmetric method [67] proceeds from the introduction of nonconjugate chiral fields $\phi_x = x + \bar{\theta}\psi$, $\phi_p = p - i\bar{\psi}\theta$ [cf. Eqn (6.26)] in which the Bose component is both the amplitude x of the hydrodynamic mode and the amplitude p of fluctuations.

According to the arguments developed above, the operators T_{\pm} that shift the time t by the Grassmann amount $\pm \bar{\theta}\theta$ transform one into another the supersymmetric fields (2.39), (2.52) and the corresponding generators (2.42), (2.53). Characteristically, only the latter of these generators are Grassmann conjugate. Such a symmetry is due to the fact that the equation of motion (2.50) is invariant with respect to the time reversion only when the conjugate force f is used, whereas equations (2.44), (2.45) which contain the amplitude φ of fluctuations are not invariant. However, apart from the superfield $\Phi_p \equiv \Phi_+$ that corresponds to $\varphi \equiv p^{(\max)}$ and is generated by the action of operator T_+ on Φ_f , the operator T_- which shifts the time in the opposite direction generates another superfield Φ_- . According to equalities (6.22), (2.24), the fields $\Phi_{\pm} \equiv \Phi_p(\pm t)$ correspond to the reverse directions of time.

It is easy to see that the action of operators T_{\pm} preserves the invariance of equations (2.46), (2.47) for the Grassmann conjugate components $\psi(\mathbf{r}, t)$, $\bar{\psi}(\mathbf{r}, t)$. To break such invariance, we introduce the operators

$$\tilde{T}_{\pm} = \exp[\varepsilon(\delta_{\pm}\bar{\theta}\psi + \delta_{\mp}\bar{\psi}\theta)], \quad (2.58)$$

where we assume $\varepsilon \rightarrow 0$; $\delta_+ = 1$, $\delta_- = 0$ for the positive time direction, and $\delta_+ = 0$, $\delta_- = 1$ for the negative time direction. The Euler equation (2.43) for the transformed superfield $\tilde{\Phi}_{\pm} \equiv \tilde{T}_{\pm}\Phi_p$ reduces to the components

$$\dot{\eta} - \nabla^2 \eta = -\frac{\partial V}{\partial \eta} + \varphi - \varepsilon \bar{\psi} \psi, \quad (2.59)$$

$$\dot{\varphi} + \nabla^2 \varphi = \frac{\partial^2 V}{\partial \eta^2} \varphi - \frac{\partial^3 V}{\partial \eta^3} \bar{\psi} \psi + \varepsilon \bar{\psi} \dot{\psi}, \quad (2.60)$$

$$\begin{aligned} \dot{\psi} - \nabla^2 \psi = & -\frac{\partial^2 V}{\partial \eta^2} \psi - \varepsilon \left\{ \delta_- \left(\frac{\dot{\psi}}{\psi} \right) \eta \right. \\ & \left. + \delta_+ \left[(\dot{\eta} - \varphi) + \frac{\partial^2 V}{\partial \eta^2} \eta \right] \right\} \psi, \end{aligned} \quad (2.61)$$

$$\begin{aligned} \dot{\bar{\psi}} + \nabla^2 \bar{\psi} = & \frac{\partial^2 V}{\partial \eta^2} \bar{\psi} - \varepsilon \left\{ \delta_+ \left(\frac{\dot{\bar{\psi}}}{\bar{\psi}} \right) \eta \right. \\ & \left. - \delta_- \left[(\dot{\eta} - \varphi) + \frac{\partial^2 V}{\partial \eta^2} \eta \right] \right\} \bar{\psi}, \end{aligned} \quad (2.62)$$

where we have retained the terms of the first order in ε . In the limit $\varepsilon \rightarrow 0$, these equations become (2.44)–(2.47). Combining equations (2.61), (2.62) with $\varepsilon \neq 0$, for the entropy (2.48) we get

$$\dot{S} + \nabla \mathbf{j} = \mp \varepsilon F S, \quad F \equiv -\frac{\partial V}{\partial x} + 2 \frac{\partial^2 V}{\partial \eta^2} \eta, \quad (2.63)$$

where the upper sign corresponds to the positive direction of time, and the lower to the negative. For a closed system ($\nabla \mathbf{j} = 0$) the entropy S may not decrease, and the positive time arrow is only realized for the negative values of the effective force $F \equiv -\partial V/\partial \eta + 2(\partial^2 V/\partial \eta^2)\eta$. Since this force is internal for the system under consideration, this means that the corresponding force $F_{\text{ext}} \equiv -F$ of (counter)action of the thermostat will be positive.

In this way, the positive direction of time is realized if the effective potential $V(\eta)$ increases with the order parameter, and is convex. Near the equilibrium, where $\partial V/\partial \eta = 0$, we have $\eta \ll 1$ and $F \simeq 2(\partial^2 V/\partial \eta^2)\eta$, and such a situation requires that the system should be unstable: $\partial^2 V/\partial \eta^2 < 0$. In the degenerate case $\partial V/\partial \eta = 0$, $\partial^2 V/\partial \eta^2 = 0$, the effective force $F = 0$, and the derivation of the (2.63)-type equation must involve terms of higher order in ε .

2.4 Supersymmetric correlation technique

The superfield-theoretical scheme described above provides for the self-consistent treatment of the memory effects and the loss of ergodicity using the correlators of superfields (2.39), (2.52). Further we shall demonstrate that the most simple case corresponds to the employment of the two-component field (2.11).

The problem consists in the definition of the supersymmetric correlator

$$C(z, z') = \langle \Phi(z) \Phi(z') \rangle, \quad z \equiv \{\mathbf{r}, t, \bar{\theta}, \theta\}, \quad (2.64)$$

which is the average computed over distribution (2.23). First we find the bare supercorrelator $C^{(0)}(z, z')$ corresponding to the harmonic potential $V_0 = (1/2)\Phi^2$. In this case, the supersymmetric equation of motion (2.43) yields

$$L_{\mathbf{k}\omega}(\theta) C_{\mathbf{k}\omega}^{(0)}(\theta, \theta') = \delta(\theta, \theta'), \quad L \equiv 1 - \frac{1}{2}[\bar{\mathcal{D}}, \mathcal{D}], \quad (2.65)$$

where we have introduced the Grassmann δ -function

$$\delta(\theta, \theta') = (\bar{\theta} - \bar{\theta}')(\theta - \theta') \quad (2.66)$$

and carried out the space-time Fourier transformation (ω is the frequency, and \mathbf{k} is the wave vector). In the general form, the solution of equation (2.65) is written down as follows

$$C^{(0)}(\theta, \theta') = \frac{1 + (1/2)[\bar{\mathcal{D}}, \mathcal{D}]}{1 - (1/4)[\bar{\mathcal{D}}, \mathcal{D}]^2} \delta(\theta, \theta'), \quad (2.67)$$

where we have dropped the subscripts ω, \mathbf{k} . With due account for definitions (2.42), (2.66) and the equality $[\bar{\mathcal{D}}, \mathcal{D}]^2 = -4\omega^2$ that follows from (6.11), the bare supercorrelator correspond-

ing to superfield (2.39) takes on the form

$$C_{\varphi}^{(0)}(\theta, \theta') = \frac{1 + (1 - i\omega)(\bar{\theta} - \bar{\theta}')\theta - (1 + i\omega)(\bar{\theta} - \bar{\theta}')\theta'}{1 + \omega^2}. \quad (2.68)$$

According to Eqn (2.54), upon passage to superfield (2.52), the numerator acquires another summand $i\omega(\bar{\theta}\theta - \bar{\theta}'\theta')$.

Given the Grassmann structure of expression (2.68), it is further convenient to introduce the basis vectors

$$\begin{aligned} T(\theta, \theta') &= 1, & B_0(\theta, \theta') &= \bar{\theta}\theta, & B_1(\theta, \theta') &= \bar{\theta}'\theta', \\ F_0(\theta, \theta') &= -\bar{\theta}'\theta, & F_1(\theta, \theta') &= -\bar{\theta}\theta'. \end{aligned} \quad (2.69)$$

We define the functional product of arbitrary vectors $\mathbf{X}, \mathbf{Y}, \mathbf{Z}$ by the equality

$$X(\theta, \theta') = \int Y(\theta, \theta'') Z(\theta'', \theta') d^2\theta''. \quad (2.70)$$

Then the components (2.69) of the basis obey the following multiplication table (Table 1):

Table 1.

$\begin{smallmatrix} r \\ l \end{smallmatrix}$	\mathbf{T}	\mathbf{B}_0	\mathbf{B}_1	\mathbf{F}_0	\mathbf{F}_1
\mathbf{T}	0	\mathbf{T}	0	0	0
\mathbf{B}_0	0	\mathbf{B}_0	0	0	0
\mathbf{B}_1	\mathbf{T}	0	\mathbf{B}_1	0	0
\mathbf{F}_0	0	0	0	\mathbf{F}_0	0
\mathbf{F}_1	0	0	0	0	\mathbf{F}_1

In this way, vectors $\mathbf{T}, \mathbf{B}_{0,1}, \mathbf{F}_{0,1}$ form a closed basis that is convenient for decomposing the main supercorrelators of the superfield. According to Eqns (6.33), (6.36), (2.69), these decompositions acquire the form

$$C_{\varphi} = S\mathbf{T} + G_+(\mathbf{B}_0 + \mathbf{F}_0) + G_-(\mathbf{B}_1 + \mathbf{F}_1), \quad (2.71)$$

$$C_f = S\mathbf{T} + m_+\mathbf{B}_0 + m_-\mathbf{B}_1 + G_+\mathbf{F}_0 + G_-\mathbf{F}_1.$$

Here, in accordance with the Ward identity (6.32), where the first of the generators in Eqn (6.31) is used, the term proportional to $\bar{\theta}\theta'\theta'$ vanishes. From the formal standpoint, expressions (2.71) are similar to the result of decomposition of a vector in terms of Cartesian coordinates, with the distinction that the supersymmetric components (2.69) are not orthogonal.

Substituting the formulas of superfields (2.39), (2.52) into definition (2.64), for the coefficients in expansions (2.71) we get [cf. Eqns (6.34), (6.37)]

$$\begin{aligned} S &= \langle |x|^2 \rangle, & m_+ &= \langle x^* \rangle f_{\text{ext}}, & m_- &= \langle x \rangle f_{\text{ext}}^*, & f_{\text{ext}} &\equiv -f, \\ G_+ &= \langle px^* \rangle = \langle \bar{\psi} \psi^* \rangle, & G_- &= \langle xp^* \rangle = \langle \bar{\psi}^* \psi \rangle. \end{aligned} \quad (2.72)$$

Hence it follows that the quantity S is the autocorrelator of the amplitude x of the hydrodynamic mode; the quantities m_{\mp} satisfying the condition $m_+^* = m_-$ reduce to the standard definition $\eta \equiv \langle x \rangle$ of the order parameter corresponding to the external force $f_{\text{ext}} \equiv -f$. The retarded and advanced Green functions G_{\mp} give the response of the amplitude x of

the hydrodynamic mode to the amplitude p of fluctuations, and vice versa (in addition, according to the Ward identity, functions G_{\pm} define the correlator of Grassmann fields $\bar{\psi}, \psi$). Comparison between equalities (2.68), (2.71) leads to the bare correlators

$$S^{(0)} = m_{\pm}^{(0)} = (1 + \omega^2)^{-1}, \quad G_{\pm}^{(0)} = (1 \pm i\omega)^{-1}. \quad (2.73)$$

As is known [68], the Fourier transforms $G_{\mp}(\omega)$ of the retarded and advanced Green functions are analytical in the upper and lower half-planes of the complex frequency ω with the cut along the real axis ω' ; along the axis ω' itself is the jump $G_-(\omega') - G_+(\omega') = 4i \text{Im } G_-(\omega')$.

This leads to equations (6.35), (6.38) which express the fluctuation-dissipative theorem:

$$G_{\pm}(\omega) = m_{\pm}(\omega) \mp i\omega S(\omega), \quad S(\omega') = \frac{2}{\omega'} \text{Im } G_-(\omega'), \quad (2.74)$$

where the frequency ω' is purely real. Integrating the last expression in Eqn (2.74) with due account for the spectral representation

$$C(\omega) = \int_{-\infty}^{\infty} \frac{\text{Im } C(\omega')}{\omega' - \omega} \frac{d\omega'}{\pi}, \quad (2.75)$$

we find

$$S(t=0) = G_{\pm}(\omega=0) \equiv \chi, \quad (2.76)$$

where the last equality is revealed as the definition of the susceptibility χ .

Decompositions (2.71) allow the supercorrelator (2.64) to be treated as a vector in the space formed by the direct product of superfields (2.39) or (2.52). According to Eqn (2.71), the use of representation (2.39) gives rise to the pairwise combination of the basis vectors:

$$\mathbf{B}_0 + \mathbf{F}_0 \equiv \mathbf{A}, \quad \mathbf{B}_1 + \mathbf{F}_1 \equiv \mathbf{B}. \quad (2.77)$$

This allows their number to be reduced to the set $\mathbf{A}, \mathbf{B}, \mathbf{T}$ which obeys the multiplication table (Table 2; cf. Table 1).

Table 2.

$\begin{smallmatrix} r \\ l \end{smallmatrix}$	\mathbf{T}	\mathbf{A}	\mathbf{B}
\mathbf{T}	0	\mathbf{T}	0
\mathbf{A}	0	\mathbf{A}	0
\mathbf{B}	\mathbf{T}	0	\mathbf{B}

As a result, the first of the decompositions in Eqn (2.71) assumes the simple form

$$C_{\varphi} = G_+\mathbf{A} + G_-\mathbf{B} + S\mathbf{T}. \quad (2.78)$$

Observe that it only contains the retarded and advanced Green functions G_{\pm} , and the structural factor S .

It is readily seen that this decomposition can be obtained if we use the dual field (2.11) from the outset. Indeed, when comparing the equations of motion (2.19), (2.43), we see that the commutator $-(1/2)[\bar{\mathcal{D}}, \mathcal{D}]$ in Eqn (2.67) becomes the generator (2.14). Then, using the definition of the nilpotent

δ -function $\delta(\vartheta - \vartheta') = \vartheta + \vartheta'$, we get in place of Eqn (2.68):

$$C^{(0)}(\vartheta, \vartheta') = \frac{1 + (1 - i\omega)\vartheta + (1 + i\omega)\vartheta'}{1 + \omega^2}. \quad (2.79)$$

It is easy to see that the definitions [cf. Eqn (2.69)]

$$T(\vartheta, \vartheta') = 1, \quad A(\vartheta, \vartheta') = \vartheta, \quad B(\vartheta, \vartheta') = \vartheta' \quad (2.80)$$

lead to the decomposition (2.78). Thus, the use of a two-component field (2.11) yields the same results as the superfield (2.39). In particular, definitions

$$\begin{aligned} \int C(\vartheta, \vartheta'') C^{-1}(\vartheta'', \vartheta') d^2\vartheta'' &= \delta(\vartheta, \vartheta'), \\ \delta(\vartheta - \vartheta') &= \vartheta + \vartheta', \\ \mathbf{C} \mathbf{C}^{-1} &= \mathbf{A} + \mathbf{B} \end{aligned} \quad (2.81)$$

give the expression for the inverted supersymmetric correlator (2.78):

$$\mathbf{C}^{-1} = G_+^{-1} \mathbf{A} + G_-^{-1} \mathbf{B} - G_+^{-1} S G_-^{-1} \mathbf{T}. \quad (2.82)$$

Observe finally that, according to definitions (2.77), (2.69), at $\mathbf{A} \equiv \mathbf{B} \equiv 0$ the condition $\theta = \theta'$ is satisfied, and the decomposition (2.78) reduces to a conventional (non-Grassmann) quantity: $C(\theta, \theta) = C(\vartheta, \vartheta) = S$. Hence immediately follow the important equalities

$$\begin{aligned} \int C(z, z) dz &= \int S(\mathbf{r}, t; \mathbf{r}, t) d\mathbf{r} dt d^2\theta = 0, \\ \int C(\zeta, \zeta) d\zeta &= \int S(\mathbf{r}, t; \mathbf{r}, t) d\mathbf{r} dt d\vartheta = 0, \end{aligned} \quad (2.83)$$

where $z \equiv \{\mathbf{r}, t, \bar{\theta}, \theta\}$, $\zeta \equiv \{\mathbf{r}, t, \vartheta\}$. Further on, we shall demonstrate that conditions (2.83) imply the zero contribution from the ring diagrams of perturbation theory, which corresponds to the replica limit $n \rightarrow 0$ [59].

2.5 Supersymmetric perturbation theory

We start with the definition

$$C(\zeta, \zeta') = \left. \frac{\delta^2 Z\{u(\zeta)\}}{\delta u(\zeta) \delta u(\zeta')} \right|_{u=0}, \quad (2.84)$$

where the generating functional (2.6) is conveniently represented as the average

$$Z\{u\} = \left\langle \exp \left(\int \phi u d\zeta \right) \right\rangle \quad (2.85)$$

computed over the distribution [cf. Eqn (2.23)]

$$P\{\phi\} = Z^{-1} \exp(-S\{\phi\}), \quad S\{\phi\} = \int \lambda(\phi) d\zeta \quad (2.86)$$

set by the Lagrangian λ in Eqn (2.16). In the zero (harmonic) approximation, the action is represented by the quadratic form

$$S_0 = \frac{1}{2} \int \phi L \phi d\zeta, \quad L \equiv 1 + D, \quad (2.87)$$

where the generator D is given by equality (2.14). The corresponding distribution presents the supersymmetric Gaussian [cf. Eqn (2.5)]

$$P_0\{\phi\} = \left(\frac{\det |L|}{2\pi} \right)^{1/2} \exp \left\{ -\frac{1}{2} \int \phi L \phi d\zeta \right\}. \quad (2.88)$$

Hence, for the bare supercorrelator we get the expression

$$C^{(0)}(\zeta, \zeta') = L^{-1} \delta(\zeta, \zeta'), \quad \delta(\vartheta, \vartheta') \equiv \vartheta + \vartheta' \quad (2.89)$$

that reduces to Eqn (2.67) if we replace $-(1/2)[\bar{D}, D]$ by D in close agreement with Eqns (2.87), (2.14). The linear operator $\mathbf{L} \equiv (\mathbf{C}^{(0)})^{-1}$, decomposed with respect to basis (2.80), with due account for Eqn (2.82) is written as

$$\begin{aligned} \mathbf{L} &= L_+ \mathbf{A} + L_- \mathbf{B} + L \mathbf{T}, \\ L_{\pm} &= 1 \pm i\omega, \quad L = -1. \end{aligned} \quad (2.90)$$

In order to go beyond the scope of zero approximation, we single out the term $S_1\{\phi\}$ corresponding to the self-action (anharmonism) in the exponential of distribution (2.86), and expand it in a power series. Then the definition (2.84) gives

$$C(\zeta, \zeta') = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \langle \phi(\zeta) (S_1\{\phi\})^n \phi(\zeta') \rangle_0, \quad (2.91)$$

where, as differentiated from Eqn (2.85), the average is computed over the bare distribution (2.88). Then, in accordance with the Wick theorem, we must uncouple expression (2.91), which in the n th order of perturbation theory gives

$$C^{(n)}(\zeta, \zeta') = \iint C^{(0)}(\zeta, \zeta_1) \Sigma^{(n)}(\zeta_1, \zeta_2) C^{(0)}(\zeta_2, \zeta') d\zeta_1 d\zeta_2. \quad (2.92)$$

Here we have introduced the supersymmetric self-energy function of the n th order, $\Sigma^{(n)}(\zeta_1, \zeta_2)$, that has to be defined. The result will depend considerably on the form of the self-action potential. Let us consider the most popular models.

2.5.1 ϕ^4 model. Here, the self-action potential assumes the form

$$V_1(\zeta) = \frac{\lambda}{4!} \phi^4(\zeta), \quad \zeta \equiv \{\mathbf{r}, t, \vartheta\}, \quad (2.93)$$

where the anharmonism constant is $\lambda > 0$. To the two first orders, the expansion (2.91) yields

$$C^{(1)}(\zeta, \zeta') = -\frac{\lambda}{4!} \int \langle \phi(\zeta) (\phi(\zeta_1))^4 \phi(\zeta') \rangle_0 d\zeta_1, \quad (2.94)$$

$$\begin{aligned} C^{(2)}(\zeta, \zeta') &= \frac{1}{2!} \left(-\frac{\lambda}{4!} \right)^2 \\ &\times \iint \langle \phi(\zeta) (\phi(\zeta_1))^4 (\phi(\zeta_2))^4 \phi(\zeta') \rangle_0 d\zeta_1 d\zeta_2. \end{aligned} \quad (2.95)$$

In expression (2.94), the number of possible pairings resulting from decoupling is 12, and formula (2.94) becomes

$$C^{(1)}(\zeta, \zeta') = -\frac{\lambda}{2} \int C^{(0)}(\zeta, \zeta_1) C^{(0)}(\zeta_1, \zeta_1) C^{(0)}(\zeta_1, \zeta') d\zeta_1 \equiv 0, \quad (2.96)$$

where we have taken into account equalities (2.64), (2.83). To the second order, the number of pairings is 192, and the application to the Wick theorem in Eqn (2.95) results in

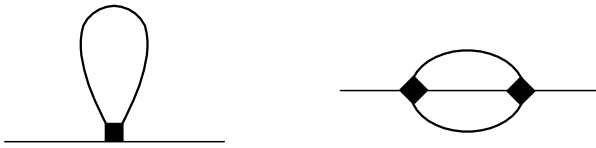
$$C^{(2)}(\zeta, \zeta') = \frac{\lambda^2}{6} \iint C^{(0)}(\zeta, \zeta_1) (C^{(0)}(\zeta_1, \zeta_2))^3 C^{(0)}(\zeta_2, \zeta') d\zeta_1 d\zeta_2. \quad (2.97)$$

According to definition (2.92), expressions (2.96), (2.97) give the supersymmetric self-energy function

$$\Sigma(\zeta, \zeta') = \frac{\lambda^2}{6} (C(\zeta, \zeta'))^3. \quad (2.98)$$

Here, in the spirit of the conventional diagram ideology, we have moved to the exact supersymmetric correlators.

In the diagram representation, expressions (2.94), (2.95) appear as



According to definition (2.83), the ring diagram vanishes, and the second diagram gives the term (2.98).

Similarly to the decomposition (2.78), it is convenient to represent the supersymmetric self-energy function in the form

$$\Sigma = \Sigma_+ \mathbf{A} + \Sigma_- \mathbf{B} + \Sigma \mathbf{T}. \quad (2.99)$$

In the determination of coefficients Σ_{\pm} , Σ one must bear in mind that the rules of multiplication in Eqn (2.98) are different from those shown in Table 2. This is because in equality (2.98) we have to use not the functional but the conventional product of dual fields [59]. The corresponding multiplication table looks like

Table 3.

	$T(\vartheta, \vartheta')$	$A(\vartheta, \vartheta')$	$B(\vartheta, \vartheta')$
$T(\vartheta, \vartheta')$	$T(\vartheta, \vartheta')$	$A(\vartheta, \vartheta')$	$B(\vartheta, \vartheta')$
$A(\vartheta, \vartheta')$	$A(\vartheta, \vartheta')$	0	0
$B(\vartheta, \vartheta')$	$B(\vartheta, \vartheta')$	0	0

As a result, for the components of decomposition (2.99) we get

$$\Sigma(t) = \frac{\lambda^2}{6} S^3(t), \quad (2.100)$$

$$\Sigma_{\pm}(t) = \frac{\lambda^2}{2} S^2(t) G_{\pm}(t). \quad (2.101)$$

Further we shall need the frequency representation, in which equations (2.100), (2.101) become

$$\Sigma(\omega) = \frac{\lambda^2}{6} \int S(\omega - \omega_1 - \omega_2) S(\omega_1) S(\omega_2) \frac{d\omega_1 d\omega_2}{(2\pi)^2}, \quad (2.102)$$

$$\Sigma_{\pm}(\omega) = \frac{\lambda^2}{2} \int G_{\pm}(\omega - \omega_1 - \omega_2) S(\omega_1) S(\omega_2) \frac{d\omega_1 d\omega_2}{(2\pi)^2}. \quad (2.103)$$

The obvious disadvantage of these expressions consists in the presence of convolutions. This problem can be avoided by using the fluctuation-dissipative theorem

$$\Sigma(t=0) = \Sigma_{\pm}(\omega=0), \quad (2.104)$$

which has the form (2.76). Then the expressions (2.100), (2.76) yield

$$\Sigma_{\pm}(\omega=0) = \frac{\lambda^2}{6} \chi^3. \quad (2.105)$$

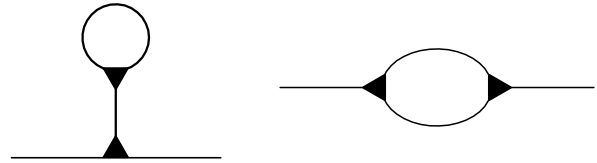
2.5.2 ϕ^3 model. Important in the theory of polymers is the cubic anharmonism set by the potential

$$V_1(\zeta) = \frac{\mu}{3!} \phi^3(\zeta), \quad \zeta = \{\mathbf{r}, t, \vartheta\}, \quad (2.106)$$

whose magnitude is determined by the parameter μ [27]. The first nonvanishing contribution to the supersymmetric correlator (2.92) assumes the form

$$C^{(2)}(\zeta', \zeta') = \frac{1}{2!} \left(-\frac{\mu}{3!} \right)^2 \times \iint \langle \phi(\zeta) (\phi(\zeta_1))^3 (\phi(\zeta_2))^3 \phi(\zeta') \rangle_0 d\zeta_1 d\zeta_2. \quad (2.107)$$

When uncoupling, it is convenient to proceed from the second-order diagrams in the form



The first of these contains a ring and, according to rule (2.83), gives a zero contribution; the second reduces to the form

$$\frac{\mu^2}{2} \iint C^{(0)}(\zeta, \zeta_1) (C^{(0)}(\zeta_1, \zeta_2))^2 C^{(0)}(\zeta_2, \zeta') d\zeta_1 d\zeta_2. \quad (2.108)$$

As a result, definition (2.92) gives rise to the expression

$$\Sigma(\zeta, \zeta') = \frac{\mu^2}{2} (C(\zeta, \zeta'))^2, \quad (2.109)$$

where the bare supersymmetric correlators are replaced with the exact correlators. Using Table 3, we get the coefficients in decomposition (2.99):

$$\Sigma(t) = \frac{\mu^2}{2} S^2(t), \quad (2.110)$$

$$\Sigma_{\pm}(t) = \mu^2 S(t) G_{\pm}(t). \quad (2.111)$$

Together with expressions (2.100), (2.101), these formulas define the supersymmetric self-energy function. Similarly to Eqn (2.105), in the ω -representation we arrive at

$$\Sigma_{\pm}(\omega=0) = \Sigma(t=0) \equiv \frac{\mu^2}{2} \chi^2. \quad (2.112)$$

In conclusion, let us report on the complete expressions for the coefficients of decomposition of the self-energy

function (2.99):

$$\Sigma(t) = \frac{1}{2} \left(\mu^2 + \frac{\lambda^2}{3} S(t) \right) S^2(t), \quad (2.113)$$

$$\Sigma_{\pm}(t) = \left(\mu^2 + \frac{\lambda^2}{2} S(t) \right) S(t) G_{\pm}(t), \quad (2.114)$$

$$\Sigma_{\pm}(\omega = 0) = \frac{1}{2} \left(\mu^2 + \frac{\lambda^2}{3} \chi \right) \chi^2. \quad (2.115)$$

2.6 Self-consistent scheme

Our next task consists in deriving the set of equations that would give a self-consistent description of the main correlators S , G_{\pm} . In the mean field theory, the solution of this problem is obtained as follows: from the effective Hamiltonian that takes into account the quenched disorder in the spread of values of the interparticle potential and the conjugate field, the quadratic component is selected, corresponding to the linear approximation in the supersymmetric field theory (Section 2.6.1). The immediate procedure of developing the self-consistent set of equations is based on the supersymmetric Dyson equation (Section 2.6.2).

2.6.1 Effective supersymmetric Lagrangian. In the site representation, the supersymmetric action is given by

$$S = S_0 + S_1 + S_{\text{int}}, \quad (2.116)$$

where the following notation was used:

$$S_0 \equiv \frac{1}{2} \sum_l \int \phi_l(t, \vartheta) [1 + D(\vartheta)] \phi_l(t, \vartheta) dt d\vartheta, \quad (2.117)$$

$$S_1 \equiv \sum_l \int V_1(\phi_l(t, \vartheta)) dt d\vartheta, \quad (2.118)$$

$$S_{\text{int}} \equiv \iint \mathcal{V}_{\text{int}} dt dt' d\vartheta d\vartheta', \quad (2.119)$$

$$\mathcal{V}_{\text{int}} = V_{\text{int}} \{ \phi_l(t, \vartheta), \phi_l(t', \vartheta'), \phi_m(t, \vartheta), \phi_m(t', \vartheta') \} \delta(t - t'),$$

$$V_{\text{int}} \equiv V + W.$$

Here, the subscripts l, m denote the node numbers, and in the self-energy part of Eqn (2.118) we separated the kernel $V_1(\phi_l)$ that takes into account the effects of self-action and is defined by equalities (2.93), (2.106). The last term S_{int} includes the real two-particle interaction V and the effective interaction W which represents the quenched disorder. In the case of attractive interaction, for the former we have [69]

$$V = -\frac{1}{2} \sum_{lm} v_{lm} \phi_m(t, \vartheta) \phi_l(t', \vartheta') \phi_l(t', \vartheta') \phi_m(t, \vartheta) - \frac{1}{2} \sum_{lm} v_{lm} \phi_l(t, \vartheta) \phi_l(t', \vartheta') \phi_m(t, \vartheta) \phi_m(t', \vartheta'). \quad (2.120)$$

In the mean field approximation, one obtains

$$V \simeq -\frac{v}{2} C(t, \vartheta; t, \vartheta) \sum_l \phi_l(t', \vartheta') \phi_l(t', \vartheta') - \frac{v}{2} C(t, \vartheta; t', \vartheta') \sum_l \phi_l(t, \vartheta) \phi_l(t', \vartheta'). \quad (2.121)$$

Hereinafter $v \equiv \sum_m v_{lm} > 0$ is the attraction constant, and $C(t, \vartheta; t', \vartheta') \equiv \langle \phi_m(t, \vartheta) \phi_m(t', \vartheta') \rangle$ is the supersymmetric correlator written in site representation. In the Sherrington–Kirkpatrick model, the quenched disorder in the spread of values of the internodal overlap integral reduces to the effective attraction [44]

$$W = -\frac{1}{2} \sum_{lm} w_{lm} \phi_l(t, \vartheta) \phi_l(t', \vartheta') \phi_m(t, \vartheta) \phi_m(t', \vartheta'). \quad (2.122)$$

Hence, similarly to Eqn (2.121), it follows that

$$W \simeq -\frac{w}{2} C(t, \vartheta; t', \vartheta') \sum_l \phi_l(t, \vartheta) \phi_l(t', \vartheta'),$$

$$w \equiv \sum_m w_{lm} > 0. \quad (2.123)$$

In this way, if the real interaction (2.121) contains diagonal and nondiagonal supercorrelators, then quenched disorder only leads to the nondiagonal component (2.123). In the framework of the replica approach, this supersymmetric structure answers to the interreplica overlapping responsible for the spin-glass behavior [16].

Finding the action of a nonequilibrium system, one should remember that, in addition to the contribution (2.119) which leads to the effective interaction potential (2.122), quenched disorder is also possible in the spread of values of the force conjugate to the order parameter. This leads to an additional contribution to the supersymmetric action [44]:

$$\Delta S_0 = \frac{h^2}{2} \sum_l \int \phi_{l\omega}(\vartheta) \delta(\omega) \phi_{l\omega}(\vartheta) d\omega d\vartheta, \quad (2.124)$$

where ω is the frequency, and the intensity of quenched disorder is given by the expression

$$h^2 \equiv \frac{\overline{(f_l - \bar{f})^2} - (\Delta\varphi)^2}{(\Delta\varphi)^2}. \quad (2.125)$$

Here the over-line denotes averaging over a volume, f_l is the magnitude of the force in the node l , and $(\Delta\varphi)^2 \equiv \varphi_{\omega=0}^2$ are the root-mean-square fluctuations of this force.

The final expression for the supersymmetric action in the node–frequency representation becomes

$$S = \sum_l \int \lambda_{l\omega}(\vartheta) \frac{d\omega}{2\pi} d\vartheta + \sum_l \int \lambda_{l\omega}(\vartheta, \vartheta') \frac{d\omega}{2\pi} d\vartheta d\vartheta', \quad (2.126)$$

where the diagonal and nondiagonal Lagrangians are expressed by equalities

$$\lambda(\vartheta) \equiv \frac{1}{2} \phi(\vartheta) \{ [1 + D(\vartheta)] + 2\pi h^2 \delta(\omega) - vS \} \phi(\vartheta) + V_1(\phi(\vartheta)), \quad (2.127)$$

$$\lambda(\vartheta, \vartheta') \equiv -\frac{1}{2} (v + w) \phi(\vartheta) C(\vartheta, \vartheta') \phi(\vartheta'), \quad (2.128)$$

where the subscripts l, ω are dropped for brevity, and the generator D is given by Eqn (2.14).

In the case of a disordered heteropolymer, the interaction potentials retain the forms (2.120), (2.122), but the indices l, m assume the meaning of wave vectors. For the passage to wave

representation, it is sufficient to replace the indices with wave vectors \mathbf{l} , \mathbf{m} in Eqns (2.126)–(2.128), and replace the constants v , w with potentials $v \equiv \sum_{\mathbf{m}} v_{\mathbf{l}\mathbf{m}}$, $w \equiv \sum_{\mathbf{m}} w_{\mathbf{l}\mathbf{m}}$ in Eqns (2.121), (2.123), (2.127), (2.128).

2.6.2 Supersymmetric Dyson equation. The supersymmetric effective Lagrangian (2.126)–(2.128) answers to the Dyson equation

$$\mathbf{C}^{-1} = \mathbf{L} - \mathbf{\Sigma} - (v + w)\mathbf{C}. \quad (2.129)$$

Here, the supercorrelators involved are represented by decompositions (2.78), (2.99), (2.90) with respect to the supersymmetric basis (2.80). Then, in accordance with equalities (2.127), (2.128), the coefficient L in decomposition (2.90) becomes

$$L = L_0 + vS, \quad L_0 = -(1 + 2\pi h^2 \delta(\omega)). \quad (2.130)$$

Projecting the superequation (2.129) onto the axes (2.80), we find the components of the Dyson equation in the frequency representation:

$$S = \frac{(\Sigma - L_0)G_+G_-}{1 - wG_+G_-}, \quad (2.131)$$

$$G_{\pm}^{-1} + (v + w)G_{\pm} = L_{\pm} - \Sigma_{\pm}. \quad (2.132)$$

Here we have taken into account equality (2.82). These equations together with expressions (2.113)–(2.115) form a closed system that describes the self-consistent behavior of a nonequilibrium stochastic system.

2.7 Memory and nonergodicity effects

Following Edwards and Anderson [14], we introduce the memory parameter

$$q = \langle x(t = \infty)x(t = 0) \rangle. \quad (2.133)$$

Its inclusion leads to the extension of the structural factor in the time-domain representation:

$$S(t) = q + S_0(t), \quad (2.134)$$

where the component $S_0(t) \rightarrow 0$ as $t \rightarrow \infty$. In a similar way, the loss of ergodicity leads to the extension of the retarded Green function in the frequency-domain representation:

$$G_-(\omega) = A + G_{-0}(\omega). \quad (2.135)$$

The nonergodicity parameter (irreversible response)

$$A = \chi_0 - \chi \quad (2.136)$$

is given by the difference between the adiabatic Kubo susceptibility $\chi_0 \equiv G_-(\omega = 0)$ and the thermodynamic (isothermal) quantity $\chi \equiv G_-(\omega \rightarrow 0)$. While the former is expressed by the standard formula $\chi_0 = \delta\eta/(\delta f_{\text{ext}})$ (where $\eta \equiv \langle x \rangle$ is the order parameter, $f_{\text{ext}} \equiv -f$ is the external force), the definition of the latter requires using the correlation technique described in Section 2.4.

² For the definition of both susceptibilities χ_0 and χ , one can employ the common response function $G_-(\omega)$, assuming that the quantities $\chi_0 \equiv G_-(\omega = 0)$ and $\chi \equiv G_-(\omega \rightarrow 0)$ correspond to the equilibrium (macroscopic) and nonequilibrium (microscopic) states, respectively. Then in equations (2.76), (2.113)–(2.115), where the subscript 0 must be attached to the correlators, we use not the exact equality $\omega = 0$, but the passage to the limit $\omega \rightarrow 0$ [22].

With this purpose, we substitute the extended correlators (2.134), (2.135) into expressions (2.113), (2.114). Then the renormalized components of the self-energy function become

$$\Sigma(t) = \frac{1}{2} \left(\mu^2 + \frac{\lambda^2}{3} q \right) q^2 + \left(\mu^2 + \frac{\lambda^2}{2} q \right) q S_0(t) + \Sigma_0(t), \quad (2.137)$$

$$\Sigma_0(t) \equiv \frac{1}{2} (\mu^2 + \lambda^2 q) S_0^2(t) + \frac{\lambda^2}{6} S_0^3(t);$$

$$\Sigma_{\pm}(t) = \left(\mu^2 + \frac{\lambda^2}{2} q \right) q [A + G_{\pm 0}(t)] + \Sigma_{\pm 0}(t), \quad (2.138)$$

$$\Sigma_{\pm 0}(t) \equiv (\mu^2 + \lambda^2 q) S_0(t) G_{\pm 0}(t) + \frac{\lambda^2}{2} S_0^2(t) G_{\pm 0}(t).$$

These expressions are written down in such a way that the terms nonlinear with respect to the correlators S_0 , $G_{\pm 0}$ are collected in the expressions for Σ_0 , $\Sigma_{\pm 0}$, whereas the terms that go first vanish in the absence of memory ($q = 0$). In addition, we have dropped the terms containing $S_0 A \simeq 0$.

Substituting Fourier transforms of expressions (2.134), (2.137) into the Dyson equation (2.131) and using (2.130), we get in the ω -representation:

$$q_0 \left[1 - w\chi_0^2 - \frac{1}{2} \left(\mu^2 + \frac{\lambda^2}{3} q_0 \right) q_0 \chi_0^2 \right] = h^2 \chi_0^2, \quad (2.139)$$

$$S_0 = \frac{(1 + \Sigma_0)G_+G_-}{1 - [w + (\mu^2 + \lambda^2 q/2)q]G_+G_-}. \quad (2.140)$$

The first of these equalities corresponds to the memory-attributed δ -shaped contribution at the frequency $\omega = 0$ (as denoted by the subscript 0), and the second to $\omega \neq 0$. In the limit $\omega \rightarrow 0$, the characteristic product is $G_+G_- \rightarrow \chi^2$, and the pole of the structural factor (2.140) defines the point of ergodicity loss:

$$w + \left(\mu^2 + \frac{\lambda^2}{2} q_0 \right) q_0 = \chi_0^{-2}. \quad (2.141)$$

Going over to the ω -representation in Eqn (2.138), from relation (2.132) we get the equation for the retarded Green function:

$$G_-^{-1} + \left[(v + w) + \left(\mu^2 + \frac{\lambda^2}{2} q \right) q \right] G_- + \Sigma_{-0} - (1 - i\omega) = 0. \quad (2.142)$$

Given expression (2.115), for the determination of thermodynamic susceptibility $\chi \equiv G_-(\omega \rightarrow 0)$ follows the equation

$$1 - \chi + (v + w)\chi^2 + \frac{\mu^2}{2} \chi[(\chi + q)^2 - q^2] + \frac{\lambda^2}{6} \chi[(\chi + q)^3 - q^3] = 0. \quad (2.143)$$

The memory parameter q_0 is found in that case from the equation

$$\left(\frac{\mu^2}{2} + \frac{\lambda^2}{3} q_0 \right) q_0^2 = h^2, \quad (2.144)$$

which follows from equations (2.139), (2.141).

2.8 Analysis of equations for the memory and nonergodicity parameters

The set of equations (2.139), (2.143), (2.141), (2.136), (2.144) allows one to give a complete description of a nonergodic system with quenched disorder. The first two of the above equations are the Sherrington–Kirkpatrick equations for the adiabatic (χ_0) and isothermal (χ) susceptibilities and the corresponding memory parameters q_0 , q [16]. Equation (2.141) defines the point T_0 of ergodicity loss, equation (2.136) defines the parameter Δ of nonergodicity, and equation (2.144) gives the memory parameter q_0 conditional on the quenched disorder h . As indicated above, in the nonergodic state one must distinguish among the macroscopic (q_0 , χ_0) and the microscopic (q , χ) quantities (the former correspond to the frequency $\omega = 0$, and the latter to the limit $\omega \rightarrow 0$). One feature of such a hierarchy is that the macroscopic quantities depend on the amplitude h of quenched disorder, and the microscopic quantities depend on the temperature T . Because of this, for the definition of macroscopic parameters q_0 , χ_0 in the nonergodic state one must fix the temperature T by the value $T_0(h)$ in the curve of ergodicity loss, and for the definition of microscopic parameters q , χ , the amplitude h of quenched disorder must be taken equal to the corresponding value $h_0(T)$.

In this way, in the ergodic state, where the macroscopic values coincide with the microscopic values, the set of equations (2.139), (2.143) is found to be sufficient for the definition of the memory parameter $q \equiv q_0$ and the susceptibility $\chi \equiv \chi_0$, and the addition of equation (2.141) defines the temperature $T_0(h)$ of ergodicity loss. Upon transition to the nonergodic state, the macroscopic quantities q_0 , χ_0 retain their values $q_0(h_0)$, $\chi_0(T_0)$ corresponding to the point of ergodicity loss, and there is only one equation (2.143) left for finding the microscopic quantities q , χ . It must be supplemented with an equation of the type (2.139):

$$q \left[1 - w\chi_0^2 - \frac{1}{2} \left(\mu^2 + \frac{\lambda^2}{3} q \right) q\chi_0^2 \right] = h^2\chi_0^2, \quad (2.145)$$

where the memory parameter q assumes a microscopic character. In line with the idea of the infinite hierarchy of relaxation times [45], this equation corresponds to the microscopic level of hierarchy that is the closest to the macroscopic level.

In these equations, the quantity h , the anharmonism parameters λ , μ and interaction parameters v , w , as well as the inverse susceptibility χ^{-1} , are measured in units of temperature T . Let us now go over to the physical units of measurement for T , h , v , w , χ , q :

$$\begin{aligned} T_s &= \left(\frac{3}{2} \right)^{3/2} \frac{\mu^4}{\lambda^3}, & h_s &= \frac{3}{2} \frac{\mu^3}{\lambda^2}, & v_s = w_s &= \left(\frac{3}{2} \right)^{-1/2} \lambda, \\ \chi_s &= \left(\frac{3}{2} \right)^{-1/2} \frac{\lambda}{\mu^2}, & q_s &= \frac{3}{2} \frac{\mu^2}{\lambda^2} \equiv u. \end{aligned} \quad (2.146)$$

As a result, our main equations become

$$\begin{aligned} (1 - uT\chi) + (v + w)T\chi^2 + \frac{\chi}{2T} [(T\chi + q)^2 - q^2] \\ + \frac{\chi}{4T} [(T\chi + q)^3 - q^3] = 0, \end{aligned} \quad (2.147)$$

$$wT + \frac{q}{2} \left(1 + \frac{q}{2} \right) + \frac{h^2}{q} = \chi_0^{-2}, \quad (2.148)$$

$$wT + \frac{q_0}{2} \left(1 + \frac{q_0}{2} \right) + \frac{h^2}{q_0} = \chi_0^{-2}, \quad (2.149)$$

$$wT_0 + q_0 \left(1 + \frac{3}{4} q_0 \right) = \chi_0^{-2}, \quad (2.150)$$

$$(1 + q_0)q_0^2 = 2h^2, \quad (2.151)$$

$$\Delta = uT(\chi_0 - \chi). \quad (2.152)$$

The pattern of behavior of the system is conditional on the parameter u introduced in the last equality in Eqn (2.146). This parameter defines the ratio of nonlinear terms of the third and fourth orders: when $u \ll 1$, the main contribution comes from the biquadratic term (2.93), and when $u \gg 1$, the cubic anharmonism (2.106) is definitive. The former case corresponds to strong quenched disorder $h \gg h_s$, and the latter to weak ($h \ll h_s$).

The dependence of the macroscopic memory parameter q_0 on the amplitude h of quenched disorder is defined by Eqn (2.151). As seen from Fig. 1, the linear portion of the curve

$$q_0 = 2^{1/2} \frac{h}{\mu}, \quad u \gg 1, \quad (2.153)$$

realized in the limit $h \ll h_s$, at $h \gg h_s$ becomes a power-law dependence

$$q_0 = 3^{1/3} \left(\frac{h}{\lambda} \right)^{2/3}, \quad u \ll 1. \quad (2.154)$$

Here, like in the subsequent equations (2.155)–(2.157), (2.159)–(2.163), we use dimensionful quantities. Simultaneous solution of equations (2.147), (2.149), (2.150), where $\chi = \chi_0$, $q = q_0$, gives the temperature $T_0(h)$ of ergodicity loss for the given field spread h . The shape of the corresponding phase diagram, which for different values of interaction

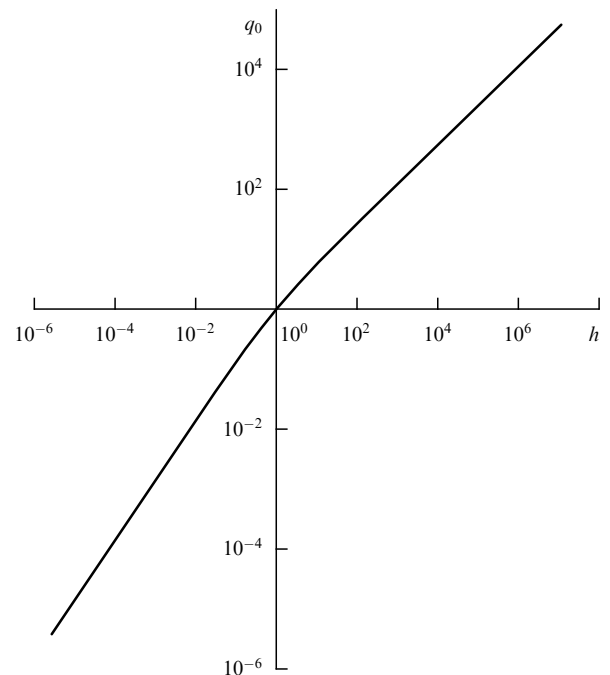


Figure 1. Macroscopic memory parameter q_0 vs. the intensity h of quenched disorder.

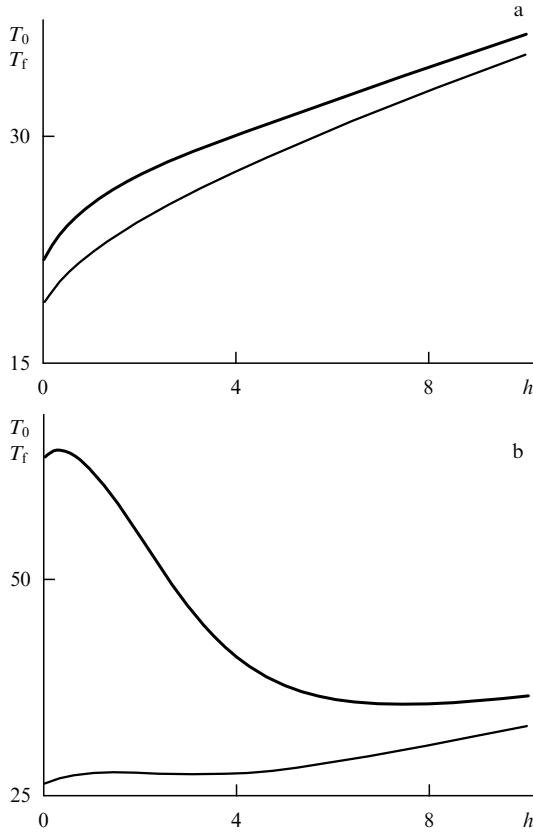


Figure 2. Temperature T_0 of ergodicity loss (thick lines) and temperature T_f of vitrification (thin lines) vs. the intensity h of quenched disorder ($u = 0.5, v = 0$) for different values of the effective parameter of interaction: $w = 0.5$ (a), $w = 0.2$ (b).

parameters w, v defines the range of the possible thermodynamic states in the $h-T$ plane, is depicted in Fig. 2. In the absence of quenched disorder h in the spread of the conjugate field, the temperature $T_{00} \equiv T_0(h=0)$ is given by

$$T_{00} = w \left\{ \left(1 + \frac{v}{2w} + \frac{1}{12} \frac{\lambda^2}{w^2} \right) + \left[\left(1 + \frac{v}{2w} + \frac{1}{12} \frac{\lambda^2}{w^2} \right)^2 + \frac{1}{2} \frac{\mu^2}{w^2} \right]^{1/2} \right\}^2 \quad (2.155)$$

and increases steadily with the increasing intensity v of interaction between particles, its dispersion w , the cubic (μ) and biquadratic (λ) anharmonicities. At large values of the amplitude h of quenched disorder, when $q_0^2 \gg q_0 \gg wT_0$, the isothermal susceptibility χ_0 in Eqn (2.150) is small, and from equations (2.147)–(2.150) it follows that $\chi_0 \approx 2/(uT_0)$. Then in the limit $\mu^2 \gg \lambda^2$ we get

$$T_0 \approx 2^{5/4} \mu \left(\frac{h}{\mu} \right)^{1/2}, \quad \left(\frac{w}{\mu} \right)^2 \mu \ll h \ll \left(\frac{\mu}{\lambda} \right)^2 \mu, \quad (2.156)$$

and for $\lambda^2 \gg \mu^2$ one finds

$$T_0 \approx 2^{1/2} 3^{1/3} \lambda \left(\frac{h}{\lambda} \right)^{2/3}, \quad h \gg \left(\frac{\mu}{\lambda} \right)^2 \mu, \quad \left(\frac{w}{\lambda} \right)^{3/2} \lambda. \quad (2.157)$$

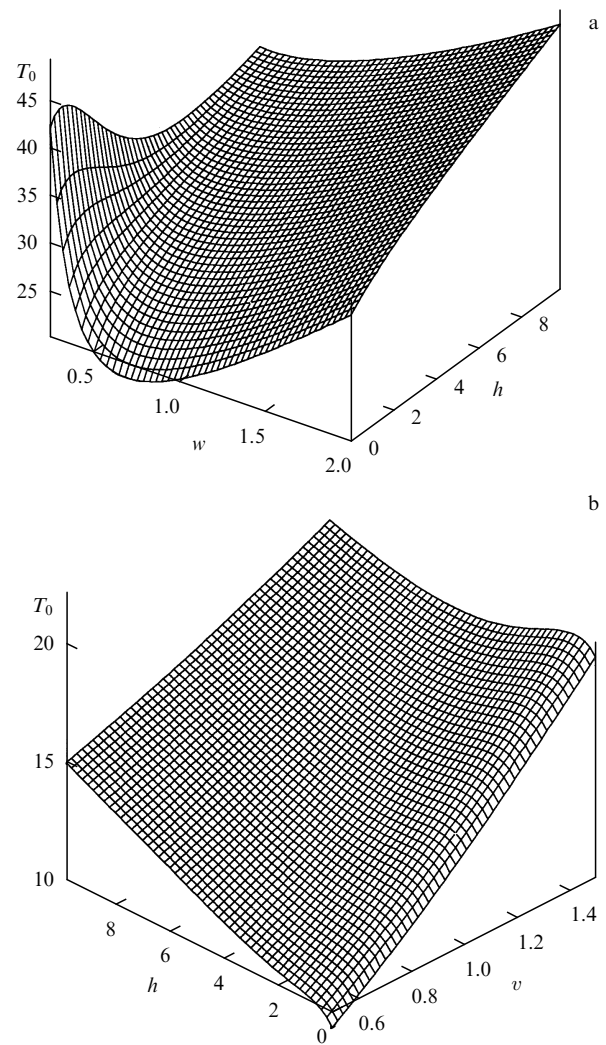


Figure 3. Temperature T_0 of ergodicity loss vs. the intensity h of quenched disorder and (a) effective interaction parameter w at $u = 0.5, v = 0$, (b) direct interaction parameter v at $u = 1, w = 0.5$.

As ought to be expected, the increase in quenched disorder intensity leads to infinite expansion of the nonergodic region. However, in the range of values of the effective interaction parameter $w < 0.5$, and also for the interaction parameter $v > 1$, the function $T_0(h)$ becomes nonmonotonic (see Figs 2 and 3).

The solution of equations (2.147)–(2.150) leads to the temperature dependences of susceptibilities χ, χ_0 shown in Fig. 4. In the nonergodic region $T < T_0$, the microscopic susceptibility χ is only nonzero at temperatures above the freezing point T_f . Its value is determined by the condition $\partial\chi/\partial T = \infty$, which together with Eqn (2.147) yields the equation

$$(v+w)T_f + T_f\chi + q + \frac{3}{4}(T_f\chi + q)^2 = \chi^{-2}, \quad (2.158)$$

where the values $\chi = \chi(T)$, $q = q(T) \equiv q_0(h_0(T))$ are taken at $T = T_f$. From Fig. 4 we see that $T_f < T_0$ always. At $h = 0$, in the limit $\mu^2, \lambda^2 \ll w^2$, we get

$$T_f \approx 4(v+w) \left[1 + \frac{\mu^2 + (2/3)\lambda^2}{4(v+w)^2} \right]. \quad (2.159)$$

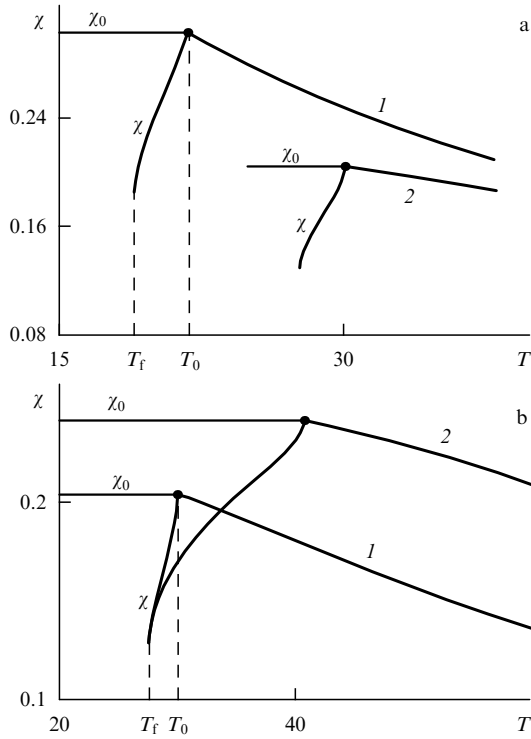


Figure 4. Temperature dependence of thermodynamic (χ) and adiabatic (χ_0) susceptibilities: (a) at $w = 0.5$, $u = 0.5$, $v = 0$, and different intensities h of quenched disorder (curves 1, 2 correspond to $h = 0, 4$); (b) at $h = 4$, $u = 0.5$, $v = 0$ and different values of the effective interaction parameter (curves 1, 2 correspond to $w = 0.5, 0.2$).

The effect of parameters w , v , u on the temperature dependence of susceptibility $\chi(T)$ is shown in Fig. 5. We see that the increase of dispersion w in the spread of interparticle interaction leads to a decrease in χ , which is accompanied by an increase in the characteristic temperatures T_{00} , T_f (Fig. 5a). A similar pattern is observed when the interaction parameter v increases (Fig. 5b), whereas the increase of parameter u has the opposite effect (Fig. 5c).

Let us finally consider the parameters of nonergodicity, Δ , and memory, q , whose values are determined by the set of equations (2.147)–(2.152). The corresponding temperature dependences are illustrated in Fig. 6. At temperatures below freezing point, where $\chi \equiv 0$ and the adiabatic susceptibility χ_0 is constant, we have a linear dependence of the nonergodicity parameter (2.152) on the temperature. The finite values of thermodynamic susceptibility χ above the freezing point T_f lead to an abrupt decrease in Δ . As the temperature further increases, the irreversible response declines steadily and goes to zero at T_0 (Fig. 6a). As the temperature increases, the microscopic memory parameter $q \equiv q_0(h_0(T))$ decreases monotonically to a minimum at the point T_0 of ergodicity loss. Above this temperature, the quantity $q_0(T)$ increases (Fig. 6b). As ought to be expected, quenched disorder expands the temperature range of nonergodicity. By analogy with phase transitions, one may assume that the microscopic memory parameter q above T_0 corresponds to the soft mode which transforms into the mode of ergodicity restoration below the temperature T_0 . Then the role of the order parameter is played by the nonergodicity parameter Δ .

Analytical expressions for the functions $\Delta(T)$, $q(T)$ can only be obtained near the curve $T_0(h)$ of ergodicity loss. At

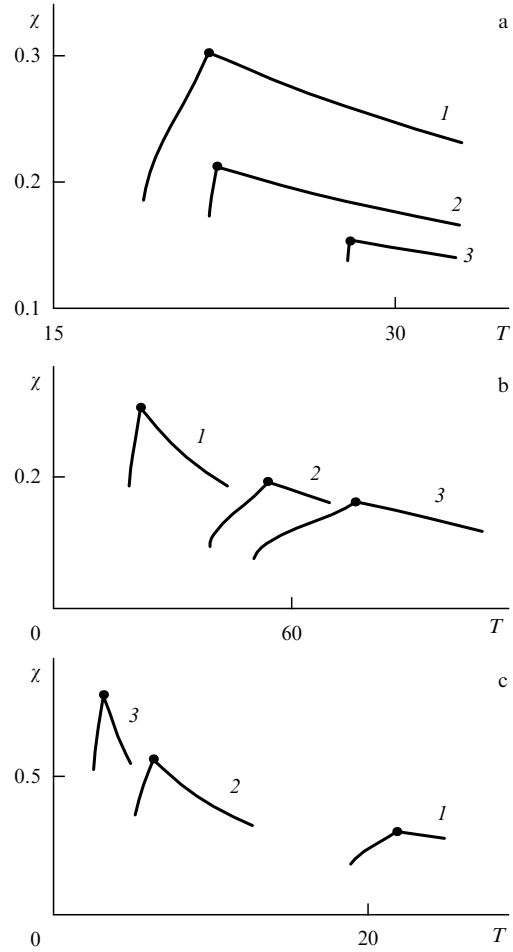


Figure 5. Shift of temperature dependences of thermodynamic susceptibility $\chi(T)$ at $h = 0$ caused by the change of (a) the effective interaction parameter w at $u = 0.5$, $v = 0$ (curves 1, 2, 3 correspond to $w = 0.5, 1, 1.5$); (b) the direct interaction parameter v at $u = 0.5$, $w = 0.5$ (curves 1, 2, 3 correspond to $v = 0, 1, 1.5$); (c) the anharmonicity ratio u at $w = 0.5$, $v = 0$ (curves 1, 2, 3 correspond to $u = 0.5, 1, 1.5$).

$h = 0$, when $T_0 = T_{00}$, from equations (2.147), where

$$|T_{00} - T| \ll T_{00}, \quad \chi \approx \chi_{00} - \frac{\Delta}{uT_{00}}, \quad \Delta \ll u\chi_{00}T_{00},$$

in the first order in $\varepsilon \equiv T/T_{00} - 1$, $(u\chi_{00}T_{00})^{-1}\Delta$ we get

$$\begin{aligned} \Delta &= -A_0\varepsilon, \quad A_0 \equiv \frac{T_{00}}{w} \left(\frac{w}{\mu} \right)^2 \\ &\times \frac{1 - \lambda^2/(6w^2)}{1 + [\lambda^2/(2\mu^2) + vw/\mu^2](T_{00}/w)^{1/2}}, \quad \varepsilon < 0; \quad (2.160) \\ q &= Q\varepsilon, \quad Q \equiv \frac{4}{3} \frac{T_{00}}{w} \left(\frac{\lambda w}{\mu^2} \right)^2 \frac{1 - \lambda^2/(12w^2)}{1 + (\lambda^2/(2\mu^2))(T_{00}/w)^{1/2}}, \quad \varepsilon > 0, \end{aligned} \quad (2.161)$$

where we have allowed for equality (2.155). In the case of $h \neq 0$, when the temperature is varied, we arrive at

$$\begin{aligned} \Delta &= -A\varepsilon, \\ A &\equiv \frac{2}{\lambda^2\chi_0^2} \frac{1 - (w/2)\chi_0^2T_0 - (\lambda^2/12)\chi_0^4T_0^2}{v/(\lambda^2\chi_0) + \mu^2/\lambda^2 + q_0 + (1/2)\chi_0T_0}, \quad \varepsilon < 0. \end{aligned} \quad (2.162)$$

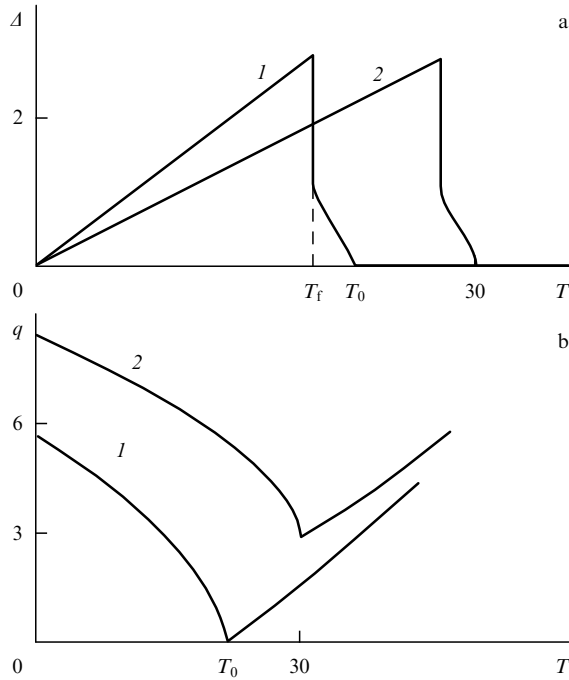


Figure 6. Temperature dependence of (a) nonergodicity parameter Δ ; (b) microscopic memory parameter q ($u = w = 0.5$, $v = 0$; curves 1, 2 correspond to $h = 0, 4$).

Accordingly, at fixed temperature in the linear approximation with respect to $q - q_0 \ll q_0$, we find

$$\Delta = B(q - q_0), \quad B^{-1} \equiv 1 + \frac{v}{\lambda^2 \chi_0} \left(\frac{\mu^2}{\lambda^2} + q_0 + \frac{1}{2} \chi_0 T_0 \right)^{-1}. \quad (2.163)$$

2.9 Incomplete loss of ergodicity

So far we have considered the steady state of a nonergodic system, which is known to take astronomically large times to reach [16]. Therefore, a real nonergodic system is always nonstationary, and one has to consider its kinetic (or, to be more precise, dynamic) behavior. Such studies have been conducted repeatedly and they affected spin glasses [45, 70, 71] and Brownian particles in a random potential [72, 73] (see also review [74]). The main object of interest are the two-time correlators that represent the memory function $C(t, t')$ and the response $R(t, t')$ (in the latter case the time t of measurement must be not less than the expectation time t').

An important feature of the nonequilibrium systems is the existence of two characteristic time regimes: the steady-state regime and the regime of annealed relaxation (aging). The former corresponds to the case considered above and is realized in the limit of the infinite expectation time $t' \rightarrow \infty$. This gives rise to the complete loss of ergodicity, defined by the irreversible response (2.152), where the adiabatic (χ_0) and isothermal (χ) susceptibilities are given by the equalities

$$\chi_0 \equiv \lim_{t-t' \rightarrow \infty} \chi(t, t'), \quad \chi \equiv \lim_{t-t' \rightarrow \infty} \lim_{t' \rightarrow \infty} \chi(t, t'),$$

$$\chi(t, t') \equiv \int_{t'}^t R(t, \tau) d\tau. \quad (2.164)$$

In addition, the system acquires memory characterized by the dynamic Edwards–Anderson parameter

$$q \equiv \lim_{t-t' \rightarrow \infty} \lim_{t' \rightarrow \infty} C(t, t'). \quad (2.165)$$

According to Ref. [45], this is conditional on the appearance of a hierarchy of infinitely high barriers that divide the phase space into isolated regions. Accordingly, the evolution of the system reduces to the conventional process of relaxation in these regions, where the property of homogeneity of time is preserved, and the fluctuation-dissipative theorem holds true for the microscopic (thermodynamic) component of the susceptibility χ defined at a given temperature T . When, however, t' decreases to finite values, the heights of these barriers go finite too, and not only the difference $t - t'$ becomes important but also the ratio $\lambda \equiv t'/t$. If the condition $t - t' \ll t' < \infty$ is satisfied, the situation reduces to our previous case $t' \rightarrow \infty$: the behavior of the system is stationary, thus being determined by the correlators $C_{st}(t - t')$, $R_{st}(t - t')$ that obey the fluctuation-dissipative theorem. It is exactly this situation that has been considered above.

As the observation time t increases to values such that $t - t' \sim t'$, we are faced with the surmount of barriers that defines the ageing process. According to Refs [70, 71], this manifests itself in that the main correlators

$$C(t, t') = C_{st}(t - t') + C_{ag}\left(\frac{t'}{t}\right),$$

$$R(t, t') = R_{st}(t - t') + t^{-1} R_{ag}\left(\frac{t'}{t}\right) \quad (2.166)$$

acquire anomalous additions $C_{ag}(t'/t)$, $t^{-1} R_{ag}(t'/t)$, for which the fluctuation-dissipative relation becomes³

$$TR_{ag}(\lambda) = X(C_{ag}(\lambda)) \frac{dC_{ag}(\lambda)}{d\lambda}, \quad \lambda \equiv \frac{t'}{t} < 1, \quad (2.167)$$

where the coefficient $X < 1$ defines the degree of deviation from normal behavior. As indicated above, such behavior is realized in the limit $t' \rightarrow \infty$, where $X \rightarrow 1$, and the integration of equality (2.167) between the limits from λ to 1 gives $T\chi_{ag}(\lambda) = C_{ag}(1) - C_{ag}(\lambda)$. Since a similar relation holds good for the stationary components, the total correlators are linked by the relation $T\chi(t, \lambda t) = C(t, t) - C(t, \lambda t)$, from which in the limits $t \rightarrow \infty$, $\lambda \rightarrow 1$ follows the linkage

$$T\chi = q(0) - q, \quad (2.168)$$

where $\chi \equiv \lim_{\lambda \rightarrow 1} \lim_{t \rightarrow \infty} \chi(t, \lambda t)$ is the thermodynamic (isothermal) susceptibility, $q \equiv \lim_{\lambda \rightarrow 1} \lim_{t \rightarrow \infty} C(t, \lambda t)$ is the Edwards–Anderson parameter [cf. definitions (2.164), (2.165)], and $q(0) \equiv C(t, t)$ is the initial value of the memory parameter.

When the condition $t - t' \sim t'$ that ensures the weak loss of ergodicity is satisfied, we have $X < 1$, and relation (2.167) leads to the definitions (2.152), (2.164) under the assumption that in the limit $t' \rightarrow \infty$, taken after the passage to the limit

³ Observe that usually this relation features total correlators rather than their nonstationary components [70–75].

$t - t' \rightarrow \infty$, we have the equality (see Ref. [75])

$$x(q) = -\frac{d\chi(\lambda)}{dq(\lambda)}, \quad \chi(\lambda) \equiv \lim_{t \rightarrow \infty} \chi(t, \lambda t),$$

$$q(\lambda) \equiv \lim_{t \rightarrow \infty} C_{ag}(t, \lambda t), \quad (2.169)$$

where the overlap parameter is $q(\lambda) < q$. Indeed, in this case the integration of expression (2.167) gives $\chi_{ag}(\lambda) = \chi(\lambda) - \chi(1)$, where the minuend corresponds to the total response function, and the subtrahend to its stationary component. This expression assumes the form of equality (2.164) if we adopt the definition $\Delta \equiv -T \lim_{\lambda \rightarrow 1} \chi_{ag}(\lambda)$ [22] and note that the macroscopic summand $\lim_{t \rightarrow \infty} \chi(t, t) \equiv \chi_0$ reduces to Kubo's adiabatic susceptibility. On the other hand, the substitution of relation (2.169) into expression (2.167) taken in the limit $t \rightarrow \infty$ leads to a nontrivial linkage between the total susceptibility and its nonstationary component:

$$R_{ag}(\lambda) = -\lim_{t \rightarrow \infty} \frac{dR(t, \lambda t)}{d\lambda}, \quad \lim_{t \rightarrow \infty} R(t, \lambda t) = -\chi_{ag}(\lambda). \quad (2.170)$$

Similarly to the linkage between Fourier transforms of the response function R and the relaxation function χ in stationary systems, the last of these equalities presents the dispersion relation

$$R(t, t') = -\int_{t'}^t R_{ag}\left(\frac{t''}{t}\right) \frac{dt''}{t}. \quad (2.171)$$

As distinct from its counterpart which features not the time ratios but the frequency differences, this equality links the total and the nonstationary response functions which appear in place of the components of complex susceptibility.

Finally, let us quote the expression for the distribution function over the regions of phase space, separated by barriers, that follows from Eqn (2.169) [16, 18]:

$$P(q) \equiv \frac{dx}{dq} = -T \lim_{\lambda \rightarrow 1} \frac{d^2 \chi(\lambda)}{dq^2(\lambda)}. \quad (2.172)$$

Hence it follows that in order to define $P(q)$ one needs to know the asymptotic dependences of the susceptibility $\chi(\lambda) \equiv \lim_{t \rightarrow \infty} \chi(t, \lambda t)$ and the overlap parameter $q(\lambda) \equiv \lim_{t \rightarrow \infty} C_{ag}(t, \lambda t)$, which govern the behavior of the self-similar system [76–79].

3. The effective Hamiltonian of a disordered heteropolymer

A disordered heteropolymer makes up a statistical ensemble of monomers of different kinds, which are randomly bound in chains that assume different geometric configurations. As a result, the monomer distribution exhibits both compositional disorder (which obviously is frozen) in the alternation of different monomers along the chain and thermal disorder associated with the sorting of configurations [80]. Our task consists in the definition of the effective Hamiltonian which represents the free energy as a function of the order parameter, which in turn defines the spatial distribution of monomers of different kinds. In the framework of the generating functional method, such a problem has first been solved for a block copolymer, in which quenched disorder is absent [34, 37]. For the transition to disordered polymer, one must carry out additional averaging over the quenched disorder. This is accomplished either using the transfer matrix method [27, 38] or the replic method. According to

Refs [27, 38], quenched disorder has a minor effect on the free energy of a regular block copolymer (see Ref. [34]), whereas in the framework of the replica approach it has been demonstrated [41, 81] that the overlapping of replicas adds a negative term. Of course, such a considerable difference in the representation of free energy leads to opposite conclusions about the phase diagram of a disordered polymer: according to Ref. [81], fluctuations suppress not only the effect of microphase separation but also the effects of vitrification, found in Refs [27, 38].

Thus we see that it is necessary to define the form of the effective Hamiltonian of a disordered heteropolymer. In this section we shall demonstrate that the approaches described above are complementary rather than contradictory [47].

3.1 Generating functional

We start off with the expression

$$Z\{\psi(\mathbf{r})\} = \int \exp\left(C_2 \chi \int m^2(\mathbf{r}) d\mathbf{r}\right) \times \overline{\langle \delta(\rho(\mathbf{r}) - 1) \delta(\psi(\mathbf{r}) - m(\mathbf{r})) \rangle} Dm(\mathbf{r}), \quad (3.1)$$

whose structure includes the condition of incompressibility for the density ρ , and the definition of the order parameter m [38]. Here, $C_2 \equiv 4f(1-f)$, f is the volume fraction of one of the copolymer components, and χ is the Flory–Huggins parameter; the over-bar denotes averaging over the compositional disorder $\{\sigma_n\}$ in the alternation of segments of different kinds; the angle brackets stand for averaging over the conformations $\{\mathbf{r}(n)\}$ corresponding to the Hamiltonian of the Gaussian chain [25]:

$$\langle \dots \rangle \equiv \int \dots \exp\{-H_0[\mathbf{r}(n)]\} D\mathbf{r}(n),$$

$$H_0\{\mathbf{r}(n)\} \equiv \frac{3}{2b^2} \sum_n [\mathbf{r}(n+1) - \mathbf{r}(n)]^2, \quad (3.2)$$

and b is the length of the segment. The density $\rho = \langle \rho(\mathbf{r}) \rangle$ and the order parameter $m = \overline{\langle \psi(\mathbf{r}) \rangle}$ represent the mean values of the microscopic variables

$$\rho(\mathbf{r}) = \sum_n \delta(\mathbf{r} - \mathbf{r}(n)),$$

$$\psi(\mathbf{r}) = 2^{-1} C_2^{-1/2} \sum_n \sigma_n \delta(\mathbf{r} - \mathbf{r}(n)), \quad (3.3)$$

where summation is carried out along the chain. Representing δ -functions as continual integrals over the fields J_ρ, J_m , we bring expression (3.1) into the structure of the Laplace transform

$$Z\{m(\mathbf{r})\} = \int \exp\left(\int J_m(\mathbf{r}) m(\mathbf{r}) d\mathbf{r}\right) Z\{J_m(\mathbf{r})\} D J_m(\mathbf{r}) \quad (3.4)$$

for a statistical sum of the system under the action of field $J_m(\mathbf{r})$:

$$Z\{J_m(\mathbf{r})\} = \int \exp\left(C_2 \chi \int m^2(\mathbf{r}) d\mathbf{r}\right) Dm(\mathbf{r}) \times \int \exp(-F'\{J_\rho, J_m\}) D J_\rho, \quad (3.5)$$

$$F'\{J_\rho, J_m\} \equiv -\ln \left\langle \exp \left[- \int (J_\rho(\mathbf{r}) \rho(\mathbf{r}) + J_m(\mathbf{r}) \psi(\mathbf{r})) d\mathbf{r} \right] \right\rangle - \int J_\rho(\mathbf{r}) d\mathbf{r}. \quad (3.6)$$

Further it is convenient to go over to the fields

$$\begin{aligned} h_\rho(\mathbf{r}) &= J_\rho(\mathbf{r}) - V^{-1} \int J_\rho(\mathbf{r}) \, d\mathbf{r}, \\ h_m(\mathbf{r}) &= J_m(\mathbf{r}) - V^{-1} \int J_m(\mathbf{r}) \, d\mathbf{r} \end{aligned} \quad (3.7)$$

counted with respect to the volume-averaged values. The corresponding Fourier transforms

$$h(\mathbf{k}) = N^{-1/2} \int h(\mathbf{r}) \exp(-i\mathbf{k}\mathbf{r}) \, d\mathbf{r} \quad (3.8)$$

are defined by the wave vector \mathbf{k} and satisfy the conditions

$$h_\rho(\mathbf{k} = 0) = h_m(\mathbf{k} = 0) = 0. \quad (3.9)$$

Substitution of fields (3.7) into the free energy (3.6) brings it to the form

$$\begin{aligned} F' \{h_\rho, h_m\} &= -\ln \left\langle \exp \left[-N^{-1/2} \sum_{n\mathbf{k}} \left(\exp(-i\mathbf{k}\mathbf{r}(n)) h_\rho(\mathbf{k}) \right. \right. \right. \\ &\quad \left. \left. \left. + 2^{-1} C_2^{-1/2} \sigma_n \exp(-i\mathbf{k}\mathbf{r}(n)) h_m(\mathbf{k}) \right) \right] \right\rangle, \end{aligned} \quad (3.10)$$

where we have taken into account the equalities (3.3), (3.8), $\langle \sigma_n \rangle = 0$ and assumed that the elementary volume is $V/N = 1$.

Expanding expression (3.10) in terms of the moments of random quantities

$$\begin{aligned} \varepsilon_\rho &\equiv N^{-1/2} \sum_{n\mathbf{k}} \exp(-i\mathbf{k}\mathbf{r}(n)) h_\rho(\mathbf{k}), \\ \varepsilon_m &\equiv 2^{-1} (C_2 N)^{-1/2} \sum_{n\mathbf{k}} \sigma_n \exp(-i\mathbf{k}\mathbf{r}(n)) h_m(\mathbf{k}) \end{aligned} \quad (3.11)$$

accurately to terms of the fourth order, we get the cumulant series

$$\begin{aligned} F' \{h_\rho, h_m\} &\simeq -\frac{1}{2!} \overline{\varepsilon_\rho^2} - \frac{1}{2!} \overline{\varepsilon_m^2} + \frac{1}{3!} \overline{\varepsilon_m^3} + \frac{1}{2!} \overline{\varepsilon_\rho \varepsilon_m^2} \\ &\quad - \frac{1}{4!} \left[\overline{\varepsilon_m^4} - 3 \overline{\varepsilon_m^2}^2 \right]. \end{aligned} \quad (3.12)$$

Given the definitions (3.11), it is convenient to introduce the designations

$$\overline{\varepsilon_\rho^2} = \sum_{\mathbf{k}_1, \mathbf{k}_2} \overline{S_\rho^{(2)}(\mathbf{k}_1, \mathbf{k}_2)} h_\rho(\mathbf{k}_1) h_\rho(\mathbf{k}_2), \quad (3.13)$$

$$\overline{\varepsilon_m^2} = \sum_{\mathbf{k}_1, \mathbf{k}_2} \overline{S_m^{(2)}(\mathbf{k}_1, \mathbf{k}_2)} h_m(\mathbf{k}_1) h_m(\mathbf{k}_2), \quad (3.14)$$

$$\overline{\varepsilon_m^3} = \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3} \overline{S_m^{(3)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3)} h_m(\mathbf{k}_1) h_m(\mathbf{k}_2) h_m(\mathbf{k}_3), \quad (3.15)$$

$$\overline{\varepsilon_\rho \varepsilon_m^2} = \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3} \overline{S_{m\rho}^{(3)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3)} h_\rho(\mathbf{k}_1) h_m(\mathbf{k}_2) h_m(\mathbf{k}_3), \quad (3.16)$$

$$\overline{\varepsilon_m^4} = \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4} \overline{S_m^{(4)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4)} h_m(\mathbf{k}_1) h_m(\mathbf{k}_2) h_m(\mathbf{k}_3) h_m(\mathbf{k}_4), \quad (3.17)$$

$$\begin{aligned} \overline{\varepsilon_m^2}^2 &= \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4} \overline{S_m^{(2)}(\mathbf{k}_1, \mathbf{k}_2)} \overline{S_m^{(2)}(\mathbf{k}_3, \mathbf{k}_4)} \\ &\quad \times h_m(\mathbf{k}_1) h_m(\mathbf{k}_2) h_m(\mathbf{k}_3) h_m(\mathbf{k}_4). \end{aligned} \quad (3.18)$$

Here, by virtue of the homogeneity of the system, the correlators $S^{(i)}$ differ from zero under the condition that the sum of wave vectors in their arguments is zero:

$$S^{(2)}(\mathbf{k}_1, \mathbf{k}_2) = S^{(2)}(\mathbf{k}_1) \delta_{\mathbf{k}_2, 0}, \quad S^{(2)}(\mathbf{k}_1) \equiv S^{(2)}(\mathbf{k}_1, -\mathbf{k}_1); \quad (3.19)$$

$$S^{(3)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) = S^{(3)}(\mathbf{k}_1, \mathbf{k}_2) \delta_{\mathbf{k}_3, 0}, \quad (3.20)$$

$$S^{(3)}(\mathbf{k}_1, \mathbf{k}_2) \equiv S^{(3)}(\mathbf{k}_1, \mathbf{k}_2, -\mathbf{k}_2);$$

$$S^{(4)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4) = S^{(4)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) \delta_{\mathbf{k}_4, 0}, \quad (3.21)$$

$$S^{(4)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) \equiv S^{(4)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, -\mathbf{k}_3),$$

where we have used the notation

$$\mathbf{k}_{12} = \mathbf{k}_1 + \mathbf{k}_2, \quad \mathbf{k}_{13} = \mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3, \quad \dots$$

3.2 Configuration correlators

Consider the explicit expressions for correlators

$$S_\rho^{(2)}(\mathbf{k}_1) = N^{-1} \sum_{n_1, n_2} \left\langle \exp(i\mathbf{k}_1 [\mathbf{r}(n_2) - \mathbf{r}(n_1)]) \right\rangle, \quad (3.22)$$

$$S_m^{(2)}(\mathbf{k}_1) = (4C_2 N)^{-1} \sum_{n_1, n_2} (\sigma_{n_1} \sigma_{n_2}) \left\langle \exp(i\mathbf{k}_1 [\mathbf{r}(n_2) - \mathbf{r}(n_1)]) \right\rangle, \quad (3.23)$$

$$\begin{aligned} S_{m\rho}^{(3)}(\mathbf{k}_1, \mathbf{k}_2) &= (4C_2)^{-1} N^{-3/2} \sum_{n_1, n_2, n_3} (\sigma_{n_1} \sigma_{n_2} + \sigma_{n_2} \sigma_{n_3} + \sigma_{n_3} \sigma_{n_1}) \\ &\quad \times \left\langle \exp(i\mathbf{k}_1 [\mathbf{r}(n_2) - \mathbf{r}(n_1)]) \exp(i\mathbf{k}_2 [\mathbf{r}(n_3) - \mathbf{r}(n_2)]) \right\rangle, \end{aligned} \quad (3.24)$$

$$\begin{aligned} S_m^{(3)}(\mathbf{k}_1, \mathbf{k}_2) &= (4C_2 N)^{-3/2} \sum_{n_1, n_2, n_3} (\sigma_{n_1} \sigma_{n_2} \sigma_{n_3}) \\ &\quad \times \left\langle \exp(i\mathbf{k}_1 [\mathbf{r}(n_2) - \mathbf{r}(n_1)]) \exp(i\mathbf{k}_2 [\mathbf{r}(n_3) - \mathbf{r}(n_2)]) \right\rangle, \end{aligned} \quad (3.25)$$

$$\begin{aligned} S_m^{(4)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) &= (4C_2 N)^{-2} \sum_{n_1, n_2, n_3, n_4} (\sigma_{n_1} \sigma_{n_2} \sigma_{n_3} \sigma_{n_4}) \\ &\quad \times \left\langle \exp(i\mathbf{k}_1 [\mathbf{r}(n_2) - \mathbf{r}(n_1)]) \exp(i\mathbf{k}_2 [\mathbf{r}(n_3) - \mathbf{r}(n_2)]) \right. \\ &\quad \left. \times \exp(i\mathbf{k}_3 [\mathbf{r}(n_4) - \mathbf{r}(n_3)]) \right\rangle, \end{aligned} \quad (3.26)$$

$$\begin{aligned} S_m^{(2)}(\mathbf{k}_1) S_m^{(2)}(\mathbf{k}_3) &= (4C_2 N)^{-2} \sum_{n_1, n_2, n_3, n_4} (\sigma_{n_1} \sigma_{n_2} \sigma_{n_3} \sigma_{n_4}) \\ &\quad \times \left\langle \exp(i\mathbf{k}_1 [\mathbf{r}(n_2) - \mathbf{r}(n_1)]) \right\rangle \left\langle \exp(i\mathbf{k}_3 [\mathbf{r}(n_4) - \mathbf{r}(n_3)]) \right\rangle. \end{aligned} \quad (3.27)$$

Here we have regrouped the terms in the exponentials to take into account the existence of δ -shaped multipliers in the definitions (3.19)–(3.21). The configurational means reduce to pair correlators

$$\left\langle \exp(i\mathbf{k} [\mathbf{r}(n_2) - \mathbf{r}(n_1)]) \right\rangle = \exp\left(-\frac{b^2 \mathbf{k}^2}{6} |n_2 - n_1|\right), \quad (3.28)$$

the expression for which is obtained as a result of expanding the exponent in the left-hand side and taking into account that a nonzero contribution only comes from the even powers of the root-mean-square difference [25]

$$\left\langle [\mathbf{r}(n_2) - \mathbf{r}(n_1)]^2 \right\rangle = \frac{b^2}{3} |n_2 - n_1|. \quad (3.29)$$

Application of the Wick theorem in expressions (3.22)–(3.26) brings the total correlators (3.13)–(3.18) to

the form

$$\overline{S_\rho^{(2)}(\mathbf{k}_1, \mathbf{k}_2)} = N^{-1} \delta_{\mathbf{k}_{12}, \mathbf{0}} \sum_{n_1, n_2} \exp(-\mathbf{q}_1^2 |n_2 - n_1|), \quad (3.30)$$

$$\overline{S_m^{(2)}(\mathbf{k}_1, \mathbf{k}_2)} = (4C_2 N)^{-1} \delta_{\mathbf{k}_{12}, \mathbf{0}} \sum_{n_1, n_2} \overline{\sigma_{n_1} \sigma_{n_2}} \exp(-\mathbf{q}_1^2 |n_2 - n_1|), \quad (3.31)$$

$$\begin{aligned} \overline{S_{mp}^{(3)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3)} \\ = (4C_2)^{-1} N^{-3/2} \delta_{\mathbf{k}_{13}, \mathbf{0}} \sum_{n_1, n_2, n_3} (\overline{\sigma_{n_1} \sigma_{n_2}} + \overline{\sigma_{n_2} \sigma_{n_3}} + \overline{\sigma_{n_3} \sigma_{n_1}}) \\ \times \exp(-\mathbf{q}_1^2 |n_2 - n_1|) \exp(-\mathbf{q}_{12}^2 |n_3 - n_2|), \end{aligned} \quad (3.32)$$

$$\begin{aligned} \overline{S_m^{(3)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3)} = (4C_2 N)^{-3/2} \delta_{\mathbf{k}_{13}, \mathbf{0}} \sum_{n_1, n_2, n_3} \overline{\sigma_{n_1} \sigma_{n_2} \sigma_{n_3}} \\ \times \exp(-\mathbf{q}_1^2 |n_2 - n_1|) \exp(-\mathbf{q}_{12}^2 |n_3 - n_2|), \end{aligned} \quad (3.33)$$

$$\begin{aligned} \overline{S_m^{(4)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4)} = (4C_2 N)^{-2} \sum_{n_1, n_2, n_3, n_4} \overline{\sigma_{n_1} \sigma_{n_2} \sigma_{n_3} \sigma_{n_4}} \\ \times [\delta_{\mathbf{k}_{14}, \mathbf{0}} \exp(-\mathbf{q}_1^2 |n_2 - n_1|) \exp(-\mathbf{q}_{12}^2 |n_3 - n_2|) \\ \times \exp(-\mathbf{q}_{13}^2 |n_4 - n_3|) \\ + \delta_{\mathbf{k}_{1+3}, \mathbf{0}} \delta_{\mathbf{k}_{12}, \mathbf{0}} \delta_{\mathbf{k}_{34}, \mathbf{0}} \exp(-\mathbf{q}_1^2 |n_2 - n_1|) \exp(-\mathbf{q}_3^2 |n_4 - n_3|)], \end{aligned} \quad (3.34)$$

$$\begin{aligned} 3 \overline{S_m^{(2)}(\mathbf{k}_1, \mathbf{k}_2) S_m^{(2)}(\mathbf{k}_3, \mathbf{k}_4)} = \\ = (4C_2 N)^{-2} \sum_{n_1, n_2, n_3, n_4} \overline{\sigma_{n_1} \sigma_{n_2} \sigma_{n_3} \sigma_{n_4}} \delta_{\mathbf{k}_{12}, \mathbf{0}} \delta_{\mathbf{k}_{34}, \mathbf{0}} \times \\ \times (\exp(-\mathbf{q}_1^2 |n_2 - n_1|) \exp(-\mathbf{q}_3^2 |n_4 - n_3|) + \\ + \exp(-\mathbf{q}_1^2 |n_4 - n_1|) \exp(-\mathbf{q}_3^2 |n_3 - n_2|) + \\ + \exp(-\mathbf{q}_1^2 |n_3 - n_1|) \exp(-\mathbf{q}_3^2 |n_4 - n_2|)), \end{aligned} \quad (3.35)$$

where we have introduced the dimensionless wave vector $\mathbf{q} = a\mathbf{k}$, $a \equiv 6^{-1/2}b$. In uncoupling the triple correlators (3.24), (3.25) into pair and single correlators we have noted that the latter are only nonzero when the wave vector is zero. So, according to Eqns (3.7), (3.8), the contribution of such an expansion into expressions (3.15), (3.16) disappears.

The compositional correlators are given by equalities [38]:

$$\overline{\sigma_{n_1} \sigma_{n_2}} = C_2 \exp(-l^{-1} |n_2 - n_1|), \quad (3.36)$$

$$\overline{\sigma_{n_1} \sigma_{n_2} \sigma_{n_3}} = 2C_2 C_3 \exp(-l^{-1} |n_2 - n_1|) \exp(-l^{-1} |n_3 - n_2|), \quad (3.37)$$

$$\begin{aligned} \overline{\sigma_{n_1} \sigma_{n_2} \sigma_{n_3} \sigma_{n_4}} = C_2^2 \exp(-l^{-1} |n_2 - n_1|) \exp(-l^{-1} |n_4 - n_3|) \\ + 4C_2 C_3^2 \exp(-l^{-1} |n_2 - n_1|) \exp(-l^{-1} |n_3 - n_2|) \\ \times \exp(-l^{-1} |n_4 - n_3|), \end{aligned} \quad (3.38)$$

where l is the correlation length, $C_2 = 4f(1-f)$, and $C_3 = 1 - 2f$. Replacing the summation over the nodes $\{n_i\}$ of the polymer chain in Eqns (3.30)–(3.35) by integration over the total number of segments $N \gg 1$, we obtain

$$\overline{S_\rho^{(2)}(\mathbf{k}_1, \mathbf{k}_2)} = N g(N \mathbf{q}_1^2) \delta_{\mathbf{k}_{12}, \mathbf{0}}, \quad (3.39)$$

$$\overline{S_m^{(2)}(\mathbf{k}_1, \mathbf{k}_2)} = \frac{N}{4} g(N(l^{-1} + \mathbf{q}_1^2)) \delta_{\mathbf{k}_{12}, \mathbf{0}}, \quad (3.40)$$

$$\begin{aligned} \overline{S_{mp}^{(3)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3)} \\ = - \left(\frac{N}{16} \right)^{1/2} \left\{ \frac{g(N(l^{-1} + \mathbf{q}_1^2)) - g(N(l^{-1} + \mathbf{q}_{12}^2))}{\mathbf{q}_1^2 - \mathbf{q}_{12}^2} \right. \\ + \left[\frac{g(N(l^{-1} + \mathbf{q}_1^2)) - g(N \mathbf{q}_{12}^2)}{(l^{-1} + \mathbf{q}_1^2) - \mathbf{q}_{12}^2} \right. \\ + \left. \left. \frac{g(N(l^{-1} + \mathbf{q}_{12}^2)) - g(N \mathbf{q}_1^2)}{(l^{-1} + \mathbf{q}_{12}^2) - \mathbf{q}_1^2} \right] \right\} \delta_{\mathbf{k}_{13}, \mathbf{0}}, \end{aligned} \quad (3.41)$$

$$\begin{aligned} \overline{S_m^{(3)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3)} = - \frac{3}{4} \left(\frac{N}{C_2} \right)^{1/2} \\ \times C_3 \left[\frac{g(N(l^{-1} + \mathbf{q}_1^2)) - g(N(l^{-1} + \mathbf{q}_{12}^2))}{\mathbf{q}_1^2 - \mathbf{q}_{12}^2} \right] \delta_{\mathbf{k}_{13}, \mathbf{0}}, \end{aligned} \quad (3.42)$$

$$\begin{aligned} \overline{S_m^{(4)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4)} \\ = \frac{3}{4} \left\{ \left[\frac{g(N \mathbf{q}_{12}^2)}{[\mathbf{q}_{12}^2 - (l^{-1} + \mathbf{q}_1^2)][\mathbf{q}_{12}^2 - (l^{-1} + \mathbf{q}_{13}^2)]} \right. \right. \\ + (\mathbf{q}_1^2 - \mathbf{q}_{13}^2)^{-1} \left(\frac{g(N(l^{-1} + \mathbf{q}_1^2))}{(l^{-1} + \mathbf{q}_1^2) - \mathbf{q}_{12}^2} - \frac{g(N(l^{-1} + \mathbf{q}_{13}^2))}{(l^{-1} + \mathbf{q}_{13}^2) - \mathbf{q}_{12}^2} \right) \Big] \\ + 4 \frac{C_3^2}{C_2} \left(\frac{g(N(l^{-1} + \mathbf{q}_1^2))}{(\mathbf{q}_1^2 - \mathbf{q}_{12}^2)(\mathbf{q}_1^2 - \mathbf{q}_{13}^2)} + \frac{g(N(l^{-1} + \mathbf{q}_{12}^2))}{(\mathbf{q}_{12}^2 - \mathbf{q}_1^2)(\mathbf{q}_{12}^2 - \mathbf{q}_{13}^2)} \right. \\ + \left. \left. \frac{g(N(l^{-1} + \mathbf{q}_{13}^2))}{(\mathbf{q}_{13}^2 - \mathbf{q}_{12}^2)(\mathbf{q}_{13}^2 - \mathbf{q}_1^2)} \right) \right\} \delta_{\mathbf{k}_{14}, \mathbf{0}} \\ + \frac{3}{4} \left\{ \frac{1}{(l^{-1} + \mathbf{q}_1^2)(l^{-1} + \mathbf{q}_3^2)} + \frac{g(N(l^{-1} + \mathbf{q}_1^2))}{(l^{-1} + \mathbf{q}_1^2)(\mathbf{q}_1^2 - \mathbf{q}_3^2)} \right. \\ + \frac{g(N(l^{-1} + \mathbf{q}_3^2))}{(l^{-1} + \mathbf{q}_3^2)(\mathbf{q}_3^2 - \mathbf{q}_1^2)} + 4 \frac{C_3^2}{C_2} \left(\frac{g(N(l^{-1} + \mathbf{q}_1^2))}{\mathbf{q}_1^2(\mathbf{q}_1^2 - \mathbf{q}_3^2)} \right. \\ + \left. \left. \frac{g(N(l^{-1} + \mathbf{q}_3^2))}{\mathbf{q}_3^2(\mathbf{q}_3^2 - \mathbf{q}_1^2)} \right) \right\} \delta_{\mathbf{k}_{1+3}, \mathbf{0}} \delta_{\mathbf{k}_{12}, \mathbf{0}} \delta_{\mathbf{k}_{34}, \mathbf{0}}, \end{aligned} \quad (3.43)$$

$$\begin{aligned} \overline{S_m^{(2)}(\mathbf{k}_1, \mathbf{k}_2) S_m^{(2)}(\mathbf{k}_3, \mathbf{k}_4)} = \frac{1}{4} \left\{ \frac{1}{(l^{-1} + \mathbf{q}_1^2)(l^{-1} + \mathbf{q}_3^2)} \right. \\ + \frac{g(N(l^{-1} + \mathbf{q}_1^2))}{(l^{-1} + \mathbf{q}_1^2)(\mathbf{q}_1^2 - \mathbf{q}_3^2)} + \frac{g(N(l^{-1} + \mathbf{q}_3^2))}{(l^{-1} + \mathbf{q}_3^2)(\mathbf{q}_3^2 - \mathbf{q}_1^2)} \\ + \frac{g(N(\mathbf{q}_1^2 + \mathbf{q}_3^2))}{(l^{-1} - \mathbf{q}_3^2)(l^{-1} - \mathbf{q}_1^2)} + \frac{g(N(l^{-1} + \mathbf{q}_1^2))}{(l^{-1} - \mathbf{q}_3^2)(\mathbf{q}_1^2 - \mathbf{q}_3^2)} \\ + \frac{g(N(\mathbf{q}_1^2 + \mathbf{q}_3^2))}{(l^{-1} - \mathbf{q}_1^2)(l^{-1} - \mathbf{q}_3^2)} + \frac{g(N(l^{-1} + \mathbf{q}_3^2))}{(l^{-1} - \mathbf{q}_1^2)(\mathbf{q}_3^2 - \mathbf{q}_1^2)} \\ + 4 \frac{C_3^2}{C_2} \left(\frac{g(N(l^{-1} + \mathbf{q}_1^2))}{\mathbf{q}_1^2(\mathbf{q}_1^2 - \mathbf{q}_3^2)} + \frac{g(N(l^{-1} + \mathbf{q}_3^2))}{\mathbf{q}_3^2(\mathbf{q}_3^2 - \mathbf{q}_1^2)} \right. \\ + \frac{g(N(l^{-1} + \mathbf{q}_1^2 + \mathbf{q}_3^2))}{\mathbf{q}_3^2 \mathbf{q}_1^2} + \frac{g(N(l^{-1} + \mathbf{q}_1^2))}{\mathbf{q}_3^2(\mathbf{q}_3^2 - \mathbf{q}_1^2)} \\ + \left. \left. \frac{g(N(l^{-1} + \mathbf{q}_1^2 + \mathbf{q}_3^2))}{\mathbf{q}_1^2 \mathbf{q}_3^2} + \frac{g(N(l^{-1} + \mathbf{q}_3^2))}{\mathbf{q}_1^2(\mathbf{q}_1^2 - \mathbf{q}_3^2)} \right) \right\} \delta_{\mathbf{k}_{12}, \mathbf{0}} \delta_{\mathbf{k}_{34}, \mathbf{0}}. \end{aligned} \quad (3.44)$$

Here we have introduced the Debye function

$$g(x) = 2x^{-2}[\exp(-x) - 1 + x], \quad (3.45)$$

whose asymptotics are $g(x) \simeq 2/x$ at $x \gg 1$, and $g(x) \simeq 1 - x/3$ at $x \ll 1$.

3.3 Free energy

The statistical sum (3.5) is determined by the dependence $F'\{h_\rho, h_m\}$ of the free energy (3.6) on the fields (3.7). The main contribution into the integrals over the fields J_ρ, J_m in equalities (3.4), (3.5) comes from the neighborhood of a saddle point, whose position is given by the conditions

$$\frac{\delta F'}{\delta h_\rho(-\mathbf{k})} = 0, \quad \frac{\delta F'}{\delta h_m(-\mathbf{k})} = m(\mathbf{k}). \quad (3.46)$$

With due account for relations (3.12), (3.13)–(3.18), the first of these gives the stationary field

$$h_\rho(\mathbf{k}_1) = \frac{1}{2} \left(\overline{S_\rho^{(2)}(\mathbf{k}_1)} \right)^{-1} \times \sum_{\mathbf{k}_2} \overline{S_{m\rho}^{(3)}(\mathbf{k}_1, \mathbf{k}_2)} h_m(\mathbf{k}_2) h_m(-\mathbf{k}_1 - \mathbf{k}_2). \quad (3.47)$$

Substituting this expression into Eqns (3.12), (3.13)–(3.18), we find the free energy as a power series in the field h_m :

$$\begin{aligned} F'\{h_m\} &= \frac{1}{2!} \sum_{\mathbf{k}_1, \mathbf{k}_2} \gamma^{(2)}(\mathbf{k}_1, \mathbf{k}_2) h_m(\mathbf{k}_1) h_m(\mathbf{k}_2) \\ &+ \frac{1}{3!} \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3} \gamma^{(3)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) h_m(\mathbf{k}_1) h_m(\mathbf{k}_2) h_m(\mathbf{k}_3) \\ &+ \frac{1}{4!} \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4} \gamma^{(4)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4) h_m(\mathbf{k}_1) h_m(\mathbf{k}_2) h_m(\mathbf{k}_3) h_m(\mathbf{k}_4), \end{aligned} \quad (3.48)$$

where the coefficients are given by the expressions

$$\begin{aligned} \gamma^{(2)}(\mathbf{k}_1, \mathbf{k}_2) &\equiv -\overline{S_m^{(2)}(\mathbf{k}_1, \mathbf{k}_2)}, \\ \gamma^{(3)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) &\equiv \overline{S_m^{(3)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3)}, \\ \gamma^{(4)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4) &\equiv -\overline{S_m^{(4)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4)} \\ &+ 3 \left[\overline{S_m^{(2)}(\mathbf{k}_1, \mathbf{k}_2) S_m^{(2)}(\mathbf{k}_3, \mathbf{k}_4)} + \left(\overline{S_\rho^{(2)}(\mathbf{k}_1 + \mathbf{k}_2)} \right)^{-1} \right. \\ &\times \left. \overline{S_{m\rho}^{(3)}(\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_3)} \overline{S_{m\rho}^{(3)}(\mathbf{k}_3 + \mathbf{k}_4, \mathbf{k}_2)} \right] \delta_{\mathbf{k}_4, 0}. \end{aligned} \quad (3.49)$$

The corresponding dependence on the order parameter

$$\begin{aligned} F\{m\} &= \frac{1}{2!} \sum_{\mathbf{k}_1, \mathbf{k}_2} \Gamma^{(2)}(\mathbf{k}_1, \mathbf{k}_2) m(\mathbf{k}_1) m(\mathbf{k}_2) \\ &+ \frac{1}{3!} \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3} \Gamma^{(3)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) m(\mathbf{k}_1) m(\mathbf{k}_2) m(\mathbf{k}_3) \\ &+ \frac{1}{4!} \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4} \Gamma^{(4)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4) m(\mathbf{k}_1) m(\mathbf{k}_2) m(\mathbf{k}_3) m(\mathbf{k}_4) \end{aligned} \quad (3.50)$$

defines the thermodynamic potential

$$F\{m\} = F'\{h_m\} - \int h_m(\mathbf{r}) m(\mathbf{r}) d\mathbf{r}, \quad (3.51)$$

which is the Legendre transformation corresponding to the Laplace transform (3.4). Accordingly, the conjugate field assumes the form [cf. Eqn (3.46)]

$$h_m(\mathbf{k}) = -\frac{\delta F}{\delta m(-\mathbf{k})}. \quad (3.52)$$

To determine the coefficients in the expansion (3.50), one must substitute the dependence $h_m\{m\}$ [which results from this expansion and the definition (3.52)] into the inverse functional $m\{h_m\}$ which is defined by the second equality in Eqn (3.46), into which the expansion (3.48) is substituted. Comparing the coefficients with the same powers of m , in accordance with Ref. [34] we get

$$\begin{aligned} \Gamma^{(2)}(\mathbf{k}_1, \mathbf{k}_2) &= -(\gamma^{(2)}(\mathbf{k}_1, \mathbf{k}_2))^{-1}, \\ \Gamma^{(3)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) &= \gamma^{(3)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) \left(\prod_{i=1}^3 \gamma^{(2)}(\mathbf{k}_i, -\mathbf{k}_i) \right)^{-1}, \\ \Gamma^{(4)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4) &= \left[\gamma^{(4)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4) \right. \\ &\quad \left. - 3 \sum_{\mathbf{k}} \gamma^{(3)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}) (\gamma^{(2)}(\mathbf{k}, -\mathbf{k}))^{-1} \gamma^{(3)}(\mathbf{k}, \mathbf{k}_3, \mathbf{k}_4) \right] \\ &\quad \times \left(\prod_{i=1}^4 \gamma^{(2)}(\mathbf{k}_i, -\mathbf{k}_i) \right)^{-1}. \end{aligned} \quad (3.53)$$

Using equalities (3.50), (3.53), (3.49) for the effective Hamiltonian

$$\mathcal{H} = F\{m\} - C_2 \chi \sum_{\mathbf{k}} |m(\mathbf{k})|^2, \quad (3.54)$$

we arrive at the following expression

$$\begin{aligned} \mathcal{H} &= \sum_{\mathbf{k}} \tau_{\mathbf{k}} |m(\mathbf{k})|^2 + \frac{1}{2} \sum_{\mathbf{k}\mathbf{k}'} W(\mathbf{k}, \mathbf{k}') |m(\mathbf{k})|^2 |m(\mathbf{k}')|^2 \\ &- \frac{1}{3!} \sum_{\mathbf{k}_1 \mathbf{k}_2 \mathbf{k}_3} |\Gamma^{(3)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3)| m(\mathbf{k}_1) m(\mathbf{k}_2) m(\mathbf{k}_3) \\ &+ \frac{1}{4!} \sum_{\mathbf{k}_1 \mathbf{k}_2 \mathbf{k}_3 \mathbf{k}_4} \Gamma^{(4)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4) m(\mathbf{k}_1) m(\mathbf{k}_2) m(\mathbf{k}_3) m(\mathbf{k}_4), \end{aligned} \quad (3.55)$$

where

$$\begin{aligned} \tau_{\mathbf{k}} &= \left(\overline{2S_m^{(2)}(\mathbf{k})} \right)^{-1} - C_2 \chi, \\ W(\mathbf{k}, \mathbf{k}') &= \frac{1}{4} \overline{S_m^{(2)}(\mathbf{k}, -\mathbf{k}) S_m^{(2)}(\mathbf{k}', -\mathbf{k}')} \left(\prod_{i=1}^4 \overline{S_m^{(2)}(\mathbf{k}_i, -\mathbf{k}_i)} \right)^{-1}, \\ |\Gamma^{(3)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3)| &= \overline{S_m^{(3)}(\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_3)} \left(\prod_{i=1}^3 \overline{S_m^{(2)}(\mathbf{k}_i, -\mathbf{k}_i)} \right)^{-1}, \\ \Gamma^{(4)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4) &= \left\{ -\overline{S_m^{(4)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4)} \right. \\ &\quad \left. + 3 \left[\sum_{\mathbf{k}} \left(\overline{S_m^{(2)}(\mathbf{k}, -\mathbf{k})} \right)^{-1} \overline{S_m^{(3)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k})} \overline{S_m^{(3)}(\mathbf{k}, \mathbf{k}_3, \mathbf{k}_4)} \right. \right. \\ &\quad \left. \left. + \left(\overline{S_\rho^{(2)}(\mathbf{k}_1 + \mathbf{k}_2)} \right)^{-1} \overline{S_{m\rho}^{(3)}(\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_3)} \overline{S_{m\rho}^{(3)}(\mathbf{k}_3 + \mathbf{k}_4, \mathbf{k}_2)} \right] \right\} \\ &\quad \times \left(\prod_{i=1}^4 \overline{S_m^{(2)}(\mathbf{k}_i, -\mathbf{k}_i)} \right)^{-1}. \end{aligned} \quad (3.56)$$

3.4 The long-wave limit

The above expressions (3.39)–(3.44) are good for arbitrary values of wave vectors \mathbf{k} and the number of segments N . In practice, as a rule, the largest contribution comes from the long-wave region $\mathbf{k} \rightarrow 0$, and the range of values $N \gg 1$. Then the equalities (3.39)–(3.44) assume a simpler form

$$\overline{S_\rho^{(2)}(\mathbf{k})} = \frac{2}{\mathbf{q}^2}, \quad (3.57)$$

$$\overline{S_m^{(2)}(\mathbf{k})} = 2^{-1}(l^{-1} + \mathbf{q}^2)^{-1}, \quad (3.58)$$

$$\overline{S_{mp}^{(3)}(\mathbf{k}_1, \mathbf{k}_2)} = N^{-1/2} \frac{l}{2} (l + 2\mathbf{q}_1^2), \quad (3.59)$$

$$\overline{S_m^{(3)}(\mathbf{k}_1, \mathbf{k}_2)} = \frac{3}{2} (NC_2)^{-1/2} C_3 l^2, \quad (3.60)$$

$$\begin{aligned} \overline{S_m^{(4)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4)} &= \frac{3}{2} \frac{l^2}{N} \left(\mathbf{q}_{12}^2 + 4l \frac{C_3^2}{C_2} \right) \delta_{\mathbf{k}_{14}, 0} \\ &+ \frac{3}{4} l^2 \delta_{\mathbf{k}_1 + \mathbf{k}_3, 0} \delta_{\mathbf{k}_{12}, 0} \delta_{\mathbf{k}_{34}, 0}, \end{aligned} \quad (3.61)$$

$$\overline{S_m^{(2)}(\mathbf{k}_1, \mathbf{k}_2) S_m^{(2)}(\mathbf{k}_3, \mathbf{k}_4)} = l^2 \left(\frac{1}{4} + \frac{1}{N(\mathbf{q}_1^2 + \mathbf{q}_3^2)} \right) \delta_{\mathbf{k}_{12}, 0} \delta_{\mathbf{k}_{34}, 0}. \quad (3.62)$$

Substitution of these expressions into equalities (3.56) gives

$$\begin{aligned} \tau_{\mathbf{k}} &= (l^{-1} - C_2 \chi) + \mathbf{q}^2, \\ W(\mathbf{k}, \mathbf{k}') &= l^{-2} \left(1 + \frac{4}{N(\mathbf{k}^2 + \mathbf{k}'^2)} \right), \\ |I^{(3)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3)| &= \mu \equiv 12l^{-1} (NC_2)^{-1/2} C_3, \\ I^{(4)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4) &= \frac{24}{Nl} \left(1 + 5 \frac{C_3^2}{C_2} \right) \\ &- 12l^{-2} \delta_{\mathbf{k}_1 + \mathbf{k}_3, 0} \delta_{\mathbf{k}_{12}, 0} \delta_{\mathbf{k}_{34}, 0}. \end{aligned} \quad (3.63)$$

As a result, the Hamiltonian (3.54) becomes

$$\mathcal{H} = \sum_{\mathbf{k}} \tau_{\mathbf{k}} |m(\mathbf{k})|^2 + \frac{1}{2} \sum_{\mathbf{k}_1 \mathbf{k}_2} w_{\mathbf{k}_1 \mathbf{k}_2} |m(\mathbf{k}_1)|^2 |m(\mathbf{k}_2)|^2 + \int v(\mathbf{r}) d\mathbf{r}, \quad (3.64)$$

$$\tau_{\mathbf{k}} \equiv \tau + (a\mathbf{k})^2, \quad \tau \equiv l^{-1} - C_2 \chi, \quad (3.65)$$

$$w_{\mathbf{k}_1 \mathbf{k}_2} \equiv l^{-2} \left[(1 - \delta_{\mathbf{k}_1 \mathbf{k}_2}) + \frac{4}{Na^2(\mathbf{k}_1^2 + \mathbf{k}_2^2)} \right], \quad (3.66)$$

$$v = -\frac{\mu}{3!} m^3 + \frac{\lambda}{4!} m^4, \quad \mu \equiv 12C_3 C_2^{-1/2} l^{-1}, \quad (3.67)$$

Observe that if in the original expression (3.1) we neglect the δ -function that reflects the condition of incompressibility, $\rho = 1$, then the coefficient $\Gamma^{(4)}$ in expansion (3.55) acquires the form

$$\begin{aligned} \Gamma^{(4)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4) &= \frac{24}{Nl} \left(5 \frac{C_3^2}{C_2} - \frac{1}{l\mathbf{q}_{12}^2} \right) \\ &- 12l^{-2} \delta_{\mathbf{k}_1 + \mathbf{k}_3, 0} \delta_{\mathbf{k}_{12}, 0} \delta_{\mathbf{k}_{34}, 0}, \end{aligned}$$

and in the long-wave limit we have $\Gamma^{(4)} \rightarrow -\infty$. This means that the neglect of incompressibility leads, as ought to be expected, to the system instability at large values of the order parameter.

3.5 Inclusion of nonergodicity effects

The technique developed above is based on the formulas (3.36)–(3.38) which allow the correlators of quenched disorder to be expressed using the transfer matrix method [38]. More commonly used is the replica method, by which the field h_m and the order parameter m receive the replica index α , with respect to which the summation from 1 to $n \rightarrow 0$ is carried out in the Hamiltonian (3.64) [16]. Retaining in the expansion (3.12) only the term quadratic with respect to the field $h_m \Rightarrow h_\alpha$, whose steady-state value is given by the second equality in (3.46), we get

$$\begin{aligned} F\{m_\alpha\} &= \frac{1}{2} \sum_{\mathbf{k}\alpha} \left(\overline{S_{\alpha\alpha}^{(2)}(\mathbf{k})} \right)^{-1} |m_\alpha(\mathbf{k})|^2 \\ &+ \frac{1}{2} \sum_{\substack{\mathbf{k} \\ \alpha \neq \beta}} \left(\overline{S_{\alpha\beta}^{(2)}(\mathbf{k})} \right)^{-1} m_\alpha(\mathbf{k}) m_\beta(-\mathbf{k}). \end{aligned} \quad (3.68)$$

Here, the first term corresponding to the coinciding replicas $\alpha = \beta$ gives in the limit of $n \rightarrow 0$ the quadratic contribution into the expansion (3.50), and the second term describes the overlapping of replicas $\alpha \neq \beta$. The analysis of systems with quenched disorder, using the example of spin glasses, revealed that their space of states features a hierarchical structure, which is characterized by random overlapping of replicas [82]. Accordingly, the overlap parameter

$$I_{\alpha\beta}(\mathbf{k}) \equiv \left(\overline{S_{\alpha\beta}^{(2)}(\mathbf{k})} \right)^{-1}$$

in the second term of expression (3.68) is a random quantity, over which averaging has to be performed.

We shall use the simplest distribution

$$\mathcal{P}\{I_{\alpha\beta}(\mathbf{k})\} \propto \exp \left[-\frac{1}{2} \sum_{\substack{\mathbf{k}_1 \mathbf{k}_2 \\ \alpha \neq \beta}} \sigma_{\mathbf{k}_1 \mathbf{k}_2}^{-1} I_{\alpha\beta}(\mathbf{k}_1) I_{\alpha\beta}(-\mathbf{k}_2) \right] \quad (3.69)$$

characterized by the dispersion parameter $\sigma_{\mathbf{k}_1 \mathbf{k}_2}$. Then the averaging of the statistical sum $Z \equiv \exp(-F)$ adds the following term to the mean value of the free energy (3.68):

$$-\frac{1}{8} \sum_{\substack{\mathbf{k}_1 \mathbf{k}_2 \\ \alpha \neq \beta}} \sigma_{\mathbf{k}_1 \mathbf{k}_2} m_\alpha(\mathbf{k}_1) m_\beta(-\mathbf{k}_1) m_\alpha(-\mathbf{k}_2) m_\beta(\mathbf{k}_2). \quad (3.70)$$

Adding and subtracting the diagonal term with $\alpha = \beta$, we find the replica form of the Hamiltonian (3.64):

$$\begin{aligned} \mathcal{H} &= \sum_{\mathbf{k}\alpha} \tau_{\mathbf{k}} |m_\alpha(\mathbf{k})|^2 \\ &+ \frac{1}{2} \sum_{\substack{\mathbf{k}_1 \mathbf{k}_2 \\ \alpha}} \left(w_{\mathbf{k}_1 \mathbf{k}_2} + \frac{1}{4} \sigma_{\mathbf{k}_1 \mathbf{k}_2} \right) |m_\alpha(\mathbf{k}_1)|^2 |m_\alpha(\mathbf{k}_2)|^2 \\ &+ \sum_{\alpha} \int v(m_\alpha) d\mathbf{r} \\ &- \frac{1}{8} \sum_{\substack{\mathbf{k}_1 \mathbf{k}_2 \\ \alpha \neq \beta}} \sigma_{\mathbf{k}_1 \mathbf{k}_2} m_\alpha(\mathbf{k}_1) m_\beta(-\mathbf{k}_1) m_\alpha(-\mathbf{k}_2) m_\beta(\mathbf{k}_2). \end{aligned} \quad (3.71)$$

The effective Hamiltonian (3.71), which generalizes the expressions used in Refs [27, 34, 38, 41, 81], constitutes the main result of this section. Of fundamental importance here is the interreplica term, whose negative sign is the cause of the ergodicity loss in the system [16]. According to Ref. [41], the dispersion parameter $\sigma_{\mathbf{k}_1\mathbf{k}_2}$ has the same form as the second term in the potential (3.66):

$$\sigma_{\mathbf{k}_1\mathbf{k}_2} = 4l^{-2} \frac{\sigma^2}{Na^2(\mathbf{k}_1^2 + \mathbf{k}_2^2)}. \quad (3.72)$$

Another feature is the structure of the potential $w_{\mathbf{k}_1\mathbf{k}_2}$ which, differently from the potential used in Refs [27, 38], contains the first term in brackets from equality (3.66). This is associated with the existence of the multiplier $\delta_{\mathbf{k}_1+\mathbf{k}_3,0}$ in the second term of expression (3.61), which takes care of the condition $\mathbf{k}_{14} = 0$ in the definition (3.21) at $\mathbf{k}_{12} = \mathbf{k}_{34} = 0$.

3.6 Inclusion of fluctuations

A characteristic feature of the Hamiltonian (3.71) consists in the different replica structures of the even terms. The manifestation of this is that the first of these, being diagonal, leads to the renormalization of the quantity $\tau_{\mathbf{k}}$, while the nondiagonal term is responsible for the memory and non-ergodicity effects. To carry out the above renormalization (see Refs [37, 81]), we must use the mean field approximation and replace one of the multipliers $|m_{\alpha}(\mathbf{k})|^2$ by the mean value

$$G_{\mathbf{k}} = [r + c(q - q_0)^2]^{-1}, \quad q \equiv ak, \quad (3.73)$$

which represents the Green function. For a definition of the parameters r , c , q_0 , we substitute equality (3.73) into the Dyson equation:

$$G_{\mathbf{k}}^{-1} = \tau_{\mathbf{k}} + \sum_{\mathbf{k}'} u_{\mathbf{k}\mathbf{k}'} G_{\mathbf{k}'}^{-1}, \quad u_{\mathbf{k}\mathbf{k}'} \equiv w_{\mathbf{k}\mathbf{k}'} + \frac{1}{4} \sigma_{\mathbf{k}\mathbf{k}'}, \quad (3.74)$$

which corresponds to the first two terms in the Hamiltonian (3.71). Then, assuming that $u_{\mathbf{k}\mathbf{k}'} = (u^2/N)(la)^{-2}(\mathbf{k}^2 + \mathbf{k}'^2)^{-1}$ where u is a constant, we find

$$c = 2, \quad q_0^{-1} = \pi^{1/2} \frac{2}{u} l(2r)^{1/4}, \quad r = \tau + \frac{3u^2}{4\pi} \frac{l^{-2}}{\sqrt{2r}}. \quad (3.75)$$

According to the last of these equalities, the parameter r is always positive for all values falling into $-\infty < \tau < \infty$. As a result, the renormalized replica Hamiltonian (3.71) assumes the final form

$$\mathcal{H} = \sum_{\mathbf{k}\alpha} G_{\mathbf{k}}^{-1} |m_{\alpha}(\mathbf{k})|^2 + \sum_{\alpha} \int v(m_{\alpha}(\mathbf{r})) d\mathbf{r} - \frac{1}{8} \sum_{\substack{\mathbf{k}_1\mathbf{k}_2 \\ \alpha\beta}} \sigma_{\mathbf{k}_1\mathbf{k}_2} m_{\alpha}(\mathbf{k}_1) m_{\beta}(-\mathbf{k}_1) m_{\alpha}(-\mathbf{k}_2) m_{\beta}(\mathbf{k}_2). \quad (3.76)$$

3.7 Supersymmetric Hamiltonian

As found in the previous section, the replic method is equivalent to the supersymmetric approach based on the use of the field [cf. Eqn (2.39)]

$$\Phi_{\mathbf{k}}(\theta) = m(\mathbf{k}) + \bar{\psi}(\mathbf{k})\theta + \bar{\theta}\psi(\mathbf{k}) + \bar{\theta}\theta\varphi(\mathbf{k}). \quad (3.77)$$

Here, θ , $\bar{\theta}$ are the Grassmann conjugate coordinates, the quantity $\bar{\psi}(-\mathbf{k})\psi(\mathbf{k})$ defines the density of interphase bound-

aries, and $\varphi(\mathbf{k})$ is the amplitude of fluctuations. The transition from the replica Hamiltonian (3.76) to the supersymmetric Hamiltonian is accomplished by replacing the order parameter $m_{\alpha}(\mathbf{k})$ by the superfield $\Phi_{\mathbf{k}}(\theta)$. Besides, from the sum over replicas α one must go over to the integral over the supercoordinate θ . As a result, we get

$$\mathcal{H} = \int \mathcal{H}(\theta, \theta') d^2\theta d^2\theta'; \quad (3.78)$$

$$d^2\theta \equiv d\theta d\bar{\theta},$$

$$\mathcal{H}(\theta, \theta') = H(\theta)\delta(\theta - \theta') + H(\theta, \theta'),$$

$$\delta(\theta, \theta') \equiv (\bar{\theta} - \bar{\theta}')(\theta - \theta'),$$

$$H(\theta) = \sum_{\mathbf{k}} G_{\mathbf{k}}^{-1} |\Phi_{\mathbf{k}}(\theta)|^2 + \int v(\Phi(\mathbf{r}, \theta)) d\mathbf{r},$$

$$H(\theta, \theta') = -\frac{1}{8} \sum_{\mathbf{k}_1\mathbf{k}_2} \sigma_{\mathbf{k}_1\mathbf{k}_2} \Phi_{\mathbf{k}_1}(\theta) \Phi_{-\mathbf{k}_1}(\theta') \Phi_{-\mathbf{k}_2}(\theta) \Phi_{\mathbf{k}_2}(\theta').$$

From the analysis carried out in the previous section we see that the supersymmetric approach has many advantages over the replic method based on expression (3.76). Therefore, in our description of the thermodynamic properties of a disordered heteropolymer in the next section we shall use the supersymmetric Hamiltonian (3.78).

4. Supersymmetric theory of a disordered heteropolymer

As already indicated, a disordered heteropolymer constitutes a linear chain of monomers of different kinds, sometimes represented as a many letter sequence. As the temperature decreases, such a system will either suffer microphase separation like that observed in the protein biomolecules (see Refs [27, 31, 80] and references cited therein) or go into the frozen state (undergoes vitrification) [39]. This section deals with the description of the latter, based on the supersymmetric approach developed in Section 2. It is proceeded from the stochastic equation of motion which, as applied to the polymer, becomes so sophisticated that the dynamic approach is no longer powerful. Accordingly, our first task consists in finding the effective equation of motion that allows us to describe the structural features of heteropolymer exhibiting thermal and quenched disorders.

4.1 Effective equation of motion

Consider initially the simplest case of a homopolymer constituting a Gaussian chain for which the probability density of finding vector \mathbf{R} that connects the origin of the chain with N th node is given by the function $\Psi(\mathbf{R}, N)$. This function satisfies the Schrödinger equation with the imaginary time $-iN$ [25]:

$$\frac{\partial \Psi}{\partial N} = \left[D \frac{\partial^2}{\partial \mathbf{R}^2} - U(\mathbf{R}, N) \right] \Psi, \quad (4.1)$$

where the number of monomers $N \gg 1$, $D \equiv b^2/6$ is the effective diffusion coefficient determined by the length of Kuhn's segment b , and $U(\mathbf{R}, N)$ is the external field. In the limit $N \rightarrow \infty$, the solution of equation (4.1) can be represented as

$$\Psi(\mathbf{R}, N) = \int \exp \left[-\frac{S_{\mathbf{R}N} \{ \mathbf{r}(n) \}}{2D} \right] D\mathbf{r}(n), \quad (4.2)$$

where the functional integration is carried out over the function $\mathbf{r}(n)$ of the monomer coordinate versus its number in the chain; the action

$$S_{\mathbf{R}N}\{\mathbf{r}(n)\} \equiv S(\mathbf{R}, N) = \int_0^N L_0(\mathbf{r}(n)) dn \quad (4.3)$$

corresponding to the ends of the chain at the points $\mathbf{r}(0) = \mathbf{0}$ and $\mathbf{r}(N) = \mathbf{R}$ is defined by the Lagrangian of Euclidean field theory [51]:

$$L_0 = \frac{1}{2} \left(\frac{d\mathbf{r}(n)}{dn} \right)^2 + 2DU(\mathbf{r}, n). \quad (4.4)$$

Here, the first term obtained in the continual approximation $\mathbf{r}(n+1) - \mathbf{r}(n) \rightarrow d\mathbf{r}(n)/dn$ plays the role of the kinetic energy and reflects the existence of the covalent bond between the monomers in the chain [25]. Substitution of the distribution (4.2) into equation (4.1) yields an equation of Jacobi type

$$\frac{\partial S}{\partial N} = D \frac{\partial^2 S}{\partial \mathbf{R}^2} - \frac{1}{2} \left(\frac{\partial S}{\partial \mathbf{R}} \right)^2 + 2DU. \quad (4.5)$$

Introducing the generalized momentum $\mathbf{p} \equiv \partial S / \partial \mathbf{R}$ and the total derivative $d\mathbf{p}/dN \equiv \partial \mathbf{p} / \partial N + (\mathbf{p} \partial / \partial \mathbf{R}) \mathbf{p}$, we reduce the nonlinear equation (4.5) to the Burgers equation

$$\frac{d\mathbf{p}}{dN} = D \left(\frac{\partial^2 \mathbf{p}}{\partial \mathbf{R}^2} + 2 \frac{\partial U}{\partial \mathbf{R}} \right). \quad (4.6)$$

Expressions (4.1)–(4.6) form the basis for the theory of directed polymers, the kinetic theory of surface roughening, etc. (see Ref. [5]).

The Schrödinger equation (4.1) becomes the Fokker–Planck equation [63]

$$\frac{\partial P}{\partial N} = \left(D \frac{\partial^2}{\partial \mathbf{R}^2} - \frac{\partial}{\partial \mathbf{R}} \mathbf{F} \right) P, \quad (4.7)$$

if we introduce the probability

$$P(\mathbf{R}, N) = \Psi(\mathbf{R}, N) \exp \left\{ -\frac{V(\mathbf{R})}{2D} \right\}. \quad (4.8)$$

Its dependence on \mathbf{R} is determined by the effective potential

$$V \equiv - \int \mathbf{F} d\mathbf{R}. \quad (4.9)$$

Force \mathbf{F} in equation (4.7) is related to the initial potential U :

$$U = \frac{1}{4D} \mathbf{F}^2 + \frac{1}{2} \frac{\partial \mathbf{F}}{\partial \mathbf{R}}. \quad (4.10)$$

According to the theory of stochastic systems [63], the Fokker–Planck equation (4.7) corresponds to the Langevin equation

$$\frac{\partial \mathbf{R}}{\partial N} = \mathbf{F}(\mathbf{R}, N) + \zeta(N) \quad (4.11)$$

which determines the stochastic dependence $\mathbf{R} = \mathbf{R}(N)$. Here the Langevin source ζ is fixed by the conditions of white noise:

$$\langle \zeta(N) \rangle = 0, \quad \langle \zeta(N) \zeta(N') \rangle = 2D \delta(N - N'), \quad (4.12)$$

where the angle brackets denote averaging over the distribution (4.8).

To go over from the case of a homopolymer to the main object of our study, i.e. the disordered heteropolymer A-B, we need to note that stochasticity here concerns not only the spatial arrangement of monomers, but also the alternation of segments of different kinds A, B along the chain. Formally this is reflected by associating each node with the Ising variable $\theta(n)$, which takes on the value $\theta(n) = 1$ if the n th monomer is of the type A, and $\theta(n) = -1$ otherwise. As the number n of the node increases, the quantity $\theta(n)$ varies similarly to the spin reorientation in Glauber dynamics [83]. For the effective spin $\sigma(n) \equiv \theta(n) - \overline{\theta(n)}$, counted from the mean value $\overline{\theta(n)}$, the transfer matrix method leads to the correlator [38]

$$\overline{\sigma(n) \sigma(n')} = C_2 \exp \left(-\frac{|n - n'|}{l} \right), \quad (4.13)$$

$$C_2 \equiv 4f(1-f), \quad f \equiv \frac{1}{2} (1 + \overline{\theta(n)}),$$

where the over-bar denotes averaging over the compositional (quenched) disorder, l is the correlation length, and f is the fraction of monomers of the type A.

It is easy to see that the pseudospin stochastic variable $\sigma(n)$, whose correlator has the exponential form (4.13), obeys the Ornstein–Uhlenbeck equation

$$\frac{d\sigma}{dn} = -\frac{\sigma}{l} + s(n), \quad (4.14)$$

where the stochastic source $s(n)$ is represented as white noise:

$$\overline{s(n)} = 0, \quad \overline{s(n) s(n')} = \frac{2C_2}{l} \delta(n - n'). \quad (4.15)$$

According to Eqn (4.14), the linkage between the microscopic quantity $\sigma(n)$ and the stochastic variable $s(n)$ has the form of the Laplace transform

$$\sigma(n) = \int_0^n \exp \left(-\frac{n-m}{l} \right) s(m) dm. \quad (4.16)$$

Conditions (4.15) are satisfied if the white noise $s(n)$ is governed by the Gaussian distribution

$$P\{s(n)\} = \left(\frac{4\pi C_2}{l} \right)^{-1/2} \exp \left\{ -\frac{l}{4C_2} \int_0^N s^2(n) dn \right\} \quad (4.17)$$

with the intensity $4C_2 l^{-1}$ of quenched disorder. Then the order parameter, normalized to unity, is determined by the local mean

$$\eta(\mathbf{r}, n) \equiv (4C_2)^{-1/2} \overline{\sigma(n) \delta(\mathbf{r} - \mathbf{r}(n))}. \quad (4.18)$$

Hereinafter the monomer volume is taken equal to unity.

Let us find the effective equation of motion for the field (4.18). As compared with the corresponding equality (4.11), the left-hand side of the desired equation must contain the contribution $-D(\partial^2 \eta / \partial \mathbf{r}^2)$ which takes into account the presence of inhomogeneity (see Ref. [84]). Going over to the Fourier transform

$$\eta_{\mathbf{k}}(n) = N^{-1/2} \int \eta(\mathbf{r}, n) \exp(-i\mathbf{k}\mathbf{r}) d\mathbf{r}, \quad (4.19)$$

for which this inhomogeneity takes on the form $Dk^2\eta_{\mathbf{k}}$, we arrive at [cf. Eqn (2.1)]

$$\frac{\partial\eta_{\mathbf{k}}}{\partial n} + (ak)^2\eta_{\mathbf{k}} = -\frac{\partial\mathcal{H}}{\partial\eta_{\mathbf{k}}^*} + \zeta_{\mathbf{k}}. \quad (4.20)$$

Here, as before, for the effective time n we used the continual limit $n \gg 1$; the characteristic scale of the monomer is given by the renormalized length of Kuhn's segment $a \equiv D^{1/2} = 6^{-1/2}b$, and the force $f_{\mathbf{k}} = -\partial\mathcal{H}/\partial\eta_{\mathbf{k}}^*$ [cf. Eqn (4.9)] is determined by the effective Hamiltonian \mathcal{H} . Similarly to Eqn (4.12), the white noise is fixed by the conditions

$$\langle\zeta_{\mathbf{k}}\rangle = 0, \quad \langle\zeta_{\mathbf{k}}^*(n)\zeta_{\mathbf{k}'}(n')\rangle = \delta_{\mathbf{k}\mathbf{k}'}\delta(n-n'), \quad (4.21)$$

where the angle brackets denote averaging over thermal disorder.

According to Section 3, the effective Hamiltonian of the disordered heteropolymer is written in the form

$$\mathcal{H} = \sum_{\mathbf{k}} r_{\mathbf{k}} |\eta_{\mathbf{k}}|^2 - \frac{1}{2} \sum_{\mathbf{k}\mathbf{k}'} w_{\mathbf{k}\mathbf{k}'} |\eta_{\mathbf{k}}|^2 |\eta_{\mathbf{k}'}|^2 + \int v(\mathbf{r}) d\mathbf{r}; \quad (4.22)$$

$$r_{\mathbf{k}} \equiv r + 2D(k - k_0)^2, \quad r = \tau + \frac{3}{4\pi} l^{-2} (2r)^{-1/2},$$

$$\tau \equiv l^{-1} - C_2\chi, \quad k_0^{-1} \equiv 2(\pi D)^{1/2} l (2r)^{1/4};$$

$$w_{\mathbf{k}\mathbf{k}'} \equiv 4\sigma^2 l^{-2} (ND)^{-1} (\mathbf{k}^2 + \mathbf{k}'^2)^{-1}; \quad (4.23)$$

$$v \equiv -\frac{\mu}{3!} \eta^3 + \frac{\lambda}{4!} \eta^4, \quad \mu \equiv 12C_3 C_2^{-1/2} l^{-1},$$

$$\lambda \equiv 24 \left(1 + \frac{5C_3^2}{C_2}\right) l^{-1}, \quad C_2 \equiv 4f(1-f), \quad C_3 \equiv |1-2f|.$$

Its salient feature consists in the renormalization of Landau's bare parameter τ into the effective value r . This renormalization is due to the effects of fluctuations, and is only manifested when the wave number k_0 is finite. As seen from Fig. 7 showing the function $r(\tau)$, for the correlation length $l \gg 1$ at $\tau > 0$ we have $r \simeq \tau$, and at $\tau < 0$ we have $r \simeq 0$. As l decreases, the curve $r(\tau)$ becomes more flat, and is approxi-

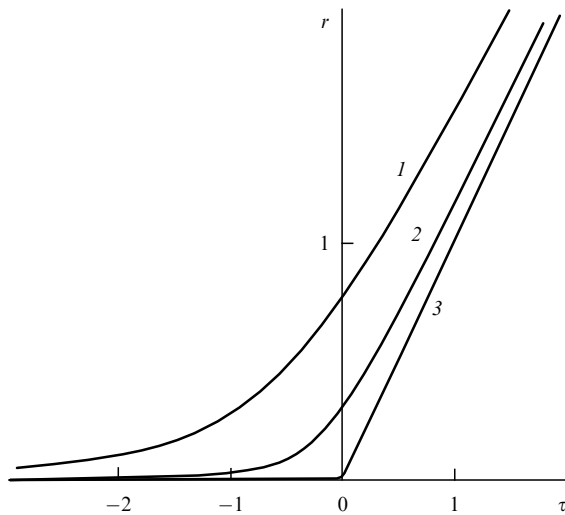


Figure 7. Renormalized parameter r vs. the bare parameter τ for different values of the correlation length l (curves 1, 2, 3 correspond to $l = 0.5, 1, 10$).

mated by the asymptotes $r \sim \tau^{-2}$ at $\tau < 0$, and $r \sim \tau$ at $\tau \gg 1$. The fundamentally new feature of this renormalization is that at all values falling within $-\infty < \tau < +\infty$ we have $r > 0$. This means that the inclusion of fluctuations converts the second-order phase transition into a first-order phase transition [36, 37].

4.2 Supersymmetric theory

Following Section 2, we start off with the generating functional

$$Z\{\eta_{\mathbf{k}}\} = \left\langle \delta\left(\frac{\partial\eta_{\mathbf{k}}}{\partial n} + \frac{\delta\mathcal{H}}{\delta\eta_{\mathbf{k}}^*} - \zeta_{\mathbf{k}}\right) \det\left|\frac{\delta\zeta_{\mathbf{k}}}{\delta\eta_{\mathbf{k}}}\right| \right\rangle, \quad (4.24)$$

$$\frac{\delta\mathcal{H}}{\delta\eta_{\mathbf{k}}^*} \equiv \frac{\partial\mathcal{H}}{\partial\eta_{\mathbf{k}}^*} + 2a^2(k - k_0)^2\eta_{\mathbf{k}},$$

where the angle brackets denote averaging over the noise $\zeta_{\mathbf{k}}(n)$, the δ -function takes into account the structure of the effective equation of motion (4.20), and the determinant gives the Jacobian of transition from the variable $\zeta_{\mathbf{k}}$ to $\eta_{\mathbf{k}}$. We write down the δ -function as the functional Laplace integral over the field $\varphi_{\mathbf{k}}(n)$ which, according to Section 2, represents the amplitude of fluctuations of the conjugate field. To bring expression (4.24) into the exponential form, we represent the determinant in terms of the Grassmann conjugate fields $\psi_{\mathbf{k}}(n)$, $\bar{\psi}_{\mathbf{k}}(n)$ [see Eqn (2.36)]. Carrying out averaging in Eqn (4.24) with respect to $\zeta_{\mathbf{k}}(n)$ and using the Gaussian distribution defined with the moments (4.21), we get

$$Z\{\eta\} = \int P\{\eta, \varphi; \psi, \bar{\psi}\} d\varphi d^2\psi,$$

$$P\{\eta, \varphi; \psi, \bar{\psi}\} = \exp(-S\{\eta, \varphi; \psi, \bar{\psi}\}), \quad S = \int_0^N \mathcal{L} dn, \quad (4.25)$$

$$\mathcal{L} = \int \left[\left(\varphi \dot{\eta} - \bar{\psi} \dot{\psi} - \frac{\varphi^2}{2} \right) + (\mathcal{H}'\{\eta\} \varphi - \bar{\psi} \mathcal{H}''\{\eta\} \psi) \right] d\mathbf{r}.$$

The dot overhead here denotes the derivative with respect to the effective time n , and the prime stands for the functional derivative over the field (4.18).

It is easy to prove by straightforward substitution that the Lagrangian corresponding to the last equality in Eqn (4.25) assumes the canonical form

$$\mathcal{L} = \int A(\Phi) d^2\theta,$$

$$A \equiv \sum_{\mathbf{k}} \frac{1}{2} (\bar{\mathcal{D}}\Phi_{\mathbf{k}}^*)(\mathcal{D}\Phi_{\mathbf{k}}) + \mathcal{H}\{\Phi_{\mathbf{k}}\}, \quad d^2\theta \equiv d\theta d\bar{\theta}; \quad (4.26)$$

$$\mathcal{D} \equiv \frac{\partial}{\partial\bar{\theta}} - 2\theta \frac{\partial}{\partial n}, \quad \bar{\mathcal{D}} \equiv \frac{\partial}{\partial\theta}$$

after the introduction of the four-component superfield [cf. Eqn (2.39)]

$$\Phi = \eta + \bar{\psi}\theta + \bar{\theta}\psi + \bar{\theta}\theta\varphi, \quad (4.27)$$

where the Grassmann coordinates $\theta, \bar{\theta}$ satisfy conditions (2.41). The functional $\mathcal{H}\{\Phi\}$ has the form (4.22), where the order parameter $\eta_{\mathbf{k}}$ is replaced with the superfield $\Phi_{\mathbf{k}}$, and the term $(\delta\mathcal{H}/\delta\eta_{\mathbf{k}}^*)\dot{\eta}_{\mathbf{k}} + \text{c.c.}$ which defines the total derivative $d\mathcal{H}\{\eta_{\mathbf{k}}(n)\}/dn$ can be dropped. According to Section 2, the combination $\bar{\psi}\psi$ corresponds to the density of interphase boundaries, and hence the employment of the four-compo-

nent superfield (4.27) corresponds to the limit of strong segregation. Further on we shall confine ourselves to the simpler case of weak segregation, which assumes that there are no boundaries altogether. According to Section 2.2, in this case the four-component superfield (4.27) reduces to the two-component (dual) form

$$\phi = \eta + \vartheta\varphi, \quad (4.28)$$

where we have introduced the self-conjugate nilpotent quantity $\vartheta \equiv \bar{\theta}\theta$. Accordingly, the Lagrangian (4.26) assumes a simple form

$$\begin{aligned} L &= \frac{1}{2} \int A(\phi) d\vartheta, \\ A &\equiv \sum_{\mathbf{k}} \phi_{\mathbf{k}}^* D \phi_{\mathbf{k}} + \mathcal{H}\{\phi_{\mathbf{k}}\}, \\ D &= -\frac{\partial}{\partial \vartheta} + \left(1 - 2\vartheta \frac{\partial}{\partial \vartheta}\right) \frac{\partial}{\partial n}. \end{aligned} \quad (4.29)$$

The equation of motion for the nilpotent field (4.28) is given by

$$D\phi_{\mathbf{k}} = -\frac{\delta \mathcal{H}}{\delta \phi_{\mathbf{k}}^*}. \quad (4.30)$$

In the componentwise form it leads to the equations of motion for the order parameter $\eta(n)$ and the amplitude of the most probable fluctuation $\varphi(n)$.

4.3 Correlation technique

We introduce now a supercorrelator of the type (2.64):

$$C_{\mathbf{k}}(n, \vartheta; n', \vartheta') \equiv \langle \phi_{\mathbf{k}}^*(n, \vartheta) \phi_{\mathbf{k}}(n', \vartheta') \rangle. \quad (4.31)$$

Multiplying the equation of motion (4.30) by $\phi_{\mathbf{k}}^*$ and averaging the result, for the bare correlator corresponding to the parameters $v = w = 0$ in the Hamiltonian (4.22) we get [cf. Eqn (2.79)]

$$C_{\mathbf{k}}^{(0)}(\vartheta, \vartheta') = \frac{1 + (r_{\mathbf{k}} - iv)\vartheta + (r_{\mathbf{k}} + iv)\vartheta'}{r_{\mathbf{k}}^2 + v^2}. \quad (4.32)$$

Here we have used the 'frequency-domain' Fourier transform

$$C_v = \int_0^N C(n) \exp(ivn) dn. \quad (4.33)$$

As found in Section 2.4, the Grassmann structure of the supercorrelator allows it to be decomposed over the basis supervectors (2.80), whose functional product obeys the rules from Table 2. According to Eqn (2.78), this decomposition is as follows

$$\mathbf{C} = G_- \mathbf{A} + G_+ \mathbf{B} + S \mathbf{T}. \quad (4.34)$$

Here and further we drop the subscripts \mathbf{k} , v for the sake of brevity. The coefficients of decomposition (4.34):

$$G_- = \langle \eta \varphi^* \rangle, \quad G_+ = \langle \eta^* \varphi \rangle, \quad S = \langle |\eta|^2 \rangle \quad (4.35)$$

are the retarded and the advanced Green functions and the structural factor, respectively. For the bare correlator $\mathbf{C}^{(0)}$

they look like

$$G_{\pm}^{(0)} = (r \pm iv)^{-1}, \quad S^{(0)} = G_+^{(0)} G_-^{(0)} = (r^2 + v^2)^{-1}. \quad (4.36)$$

The self-consistent behavior of the system is described by the Dyson equation (2.129), which for the case of a heteropolymer becomes

$$\mathbf{C}^{-1} = (\mathbf{C}^{(0)})^{-1} - w \mathbf{C} - \Sigma. \quad (4.37)$$

Here $w = 2\sigma^2(ND)^{-1}(lk_0)^{-2}$ is the characteristic value of the effective interaction potential, corresponding to the wave vectors $\mathbf{k} = \mathbf{k}' \equiv \mathbf{k}_0$ [cf. Eqn (3.72)]; Σ is the self-energy function, for which expansion (2.99) is applied. Using Eqn (4.36), we write down the components of the Dyson equation (4.37) in the form [cf. Eqns (2.131), (2.132)]

$$G_{\pm}^{-1} + w G_{\pm} = (r \pm iv) - \Sigma_{\pm}, \quad (4.38)$$

$$S = (1 + 2\pi C_2 l^{-1} \delta(v) + \Sigma) G_+ G_- (1 - w G_+ G_-)^{-1}. \quad (4.39)$$

Here the term containing the delta-function is due to the presence of quenched disorder. To close the system (4.38), (4.39), we have to express the components Σ_{\pm} , Σ of the self-energy function in terms of the components G_{\pm} , S of the supercorrelator. The supersymmetric perturbation theory presented in Section 2.5 leads to the expression

$$\begin{aligned} \Sigma(z, z') &= \frac{\mu^2}{2} \delta(z, z') \int C(z, z'') C(z'', z'') dz'' \\ &+ \frac{\mu^2}{2} (C(z, z'))^2 + \frac{\lambda^2}{6} (C(z, z'))^3, \end{aligned} \quad (4.40)$$

where $z \equiv \{\mathbf{r}, n, \vartheta\}$, $\delta(z) = \vartheta \delta(\mathbf{r}) \delta(n)$, and the product of supercorrelators is understood not in the functional but in the common sense (see Table 3). As a result, equation (4.40) gives

$$\Sigma_{\pm}(n) = \left(\mu^2 + \frac{\lambda^2}{2} S(n) \right) S(n) G_{\pm}(n), \quad (4.41)$$

$$\Sigma(n) = \frac{1}{2} \left(\mu^2 + \frac{\lambda^2}{3} S(n) \right) S^2(n). \quad (4.42)$$

Observe that here we employed the space-time representation, whereas the Dyson equations (4.38), (4.39) are written down in the frequency-wave representation.

4.4 Inclusion of memory and nonergodicity effects

Following Edwards and Anderson [14], we introduce the compositional memory parameter $q \equiv \langle \eta(n=N) \eta(n=0) \rangle$ whose magnitude determines the correlation in the alternation of monomers along the polymer chain. Also, we deduce the nonergodicity parameter $\Delta \equiv g_0 - g$ defined as the difference between the adiabatic, $g_0 \equiv G_-(v=0)$, and isothermal, $g \equiv G_-(v \rightarrow 0)$, susceptibilities. According to Section 2, the basic correlators then assume the extended form

$$G_{\pm}(v) = \Delta + G_{\pm 0}(v), \quad S(n) = q + S_0(n), \quad (4.43)$$

where the subscript 0 denotes the terms corresponding to the ergodic system without memory. Substituting the compo-

nents of Eqn (4.43) into Eqns (4.41), (4.42), we get

$$\Sigma_{\pm}(n) = \left(\mu^2 + \frac{\lambda^2}{2} q\right) q(\Delta + G_{\pm 0}(n)) + \Sigma_{\pm 0}(n), \quad (4.44)$$

$$\Sigma_{\pm 0}(n) \equiv (\mu^2 + \lambda^2 q) S_0(n) G_{\pm 0}(n) + \frac{\lambda^2}{2} S_0^2(n) G_{\pm 0}(n);$$

$$\Sigma(n) = \frac{1}{2} \left(\mu^2 + \frac{\lambda^2}{3} q\right) q^2 + \left(\mu^2 + \frac{\lambda^2}{2} q\right) q S_0(n) + \Sigma_0(n),$$

$$\Sigma_0(n) \equiv \frac{1}{2} (\mu^2 + \lambda^2 q) S_0^2(n) + \frac{\lambda^2}{6} S_0^3(n). \quad (4.45)$$

First here are those terms that vanish in the absence of memory; the contributions nonlinear with respect to correlators $G_{\pm 0}$, S_0 are brought together in the terms $\Sigma_{\pm 0}$, Σ_0 , and the product $S_0 \Delta \approx 0$ was dropped. For the transition from the time-domain representation of the self-energy function components (4.44), (4.45) to the frequency-domain representation used in the Dyson equation, we apply to the fluctuation-dissipative theorem (2.76), (2.104):

$$S_0(n \rightarrow 0) = G_{\pm 0}(v \rightarrow 0) \equiv g, \quad (4.46)$$

$$\Sigma_{\pm 0}(v \rightarrow 0) = \Sigma_0(n \rightarrow 0) \equiv \frac{1}{2} (\mu^2 + \lambda^2 q) g^2 + \frac{\lambda^2}{6} g^3, \quad (4.47)$$

where in the last equality we have accounted for Eqn (4.45)

Substituting the Fourier transforms of the components (4.43)–(4.45) into the Dyson equation (4.39), we arrive at

$$q_0 \left[1 - w g_0^2 - \frac{1}{2} \left(\mu^2 + \frac{\lambda^2}{3} q_0 \right) q_0 g_0^2 \right] = C_2 l^{-1} g_0^2, \quad (4.48)$$

$$S_0 = \frac{(1 + \Sigma_0) G_+ G_-}{1 - [w + (\mu^2 + \lambda^2 q/2) q] G_+ G_-}. \quad (4.49)$$

The first of these equations corresponds to the delta-shaped contributions and reflects the memory effects, while the second is defined when the frequency $v \neq 0$. In the limit $v \rightarrow 0$, the characteristic product exhibits $G_+ G_- \rightarrow g^2$, and the pole of structural factor (4.49)

$$w + \left(\mu^2 + \frac{\lambda^2}{2} q_0 \right) q_0 = g_0^{-2}, \quad g_0 \equiv G_-(v=0) \quad (4.50)$$

defines the point of ergodicity loss. Substituting the corresponding components (4.44) and (4.47) for the self-energy part into the Dyson equation (4.38) and using definition $g \equiv G_-(v \rightarrow 0)$, we get the equation that links the microscopic values of susceptibility and the memory parameter:

$$1 - r g + w g^2 + \frac{\mu^2}{2} g[(g+q)^2 - q^2] + \frac{\lambda^2}{6} g[(g+q)^3 - q^3] = 0. \quad (4.51)$$

The set of equations (4.48)–(4.51) describe the thermodynamic behavior of a disordered heteropolymer near the point of ergodicity loss. Like in the theory of spin glasses [16], expressions (4.48), (4.51) represent the Sherrington–Kirkpatrick equations, while condition (4.50) defines the de Ailmaida–Thouless point. According to Section 2.8, in the analysis of these equations one must distinguish between the

macroscopic and the microscopic magnitudes of the memory parameter q_0 , q and the susceptibility g_0 , g . Such a hierarchy reflects the fact that the microscopic characteristics corresponding to the limit $v \rightarrow 0$ are the ordinary thermodynamic parameters and depend on the temperature (the Flory–Huggins parameter χ). By contrast, the macroscopic quantities q_0 , g_0 correspond to $v = 0$ and depend on the quenched disorder parameter l . In the nonergodic region, the macroscopic quantities assume the values corresponding to the point of ergodicity loss.

When it comes to the behavior of these variables, the simplest is the dependence of the macroscopic memory parameter q_0 on the intensity of quenched disorder. It is described by a cubic equation which follows from equalities (4.48), (4.50):

$$\left(\frac{\mu^2}{2} + \frac{\lambda^2 q_0}{3} \right) q_0^2 = C_2 l^{-1}. \quad (4.52)$$

The characteristic curve of the macroscopic memory parameter versus the intensity of quenched disorder is depicted in Fig. 8. When the amounts of the two monomers A and B are the same ($f = 0.5$), the first term in Eqn (4.52) vanishes, and we have $q_0 \propto l^{1/3}$. In the case of a dilute copolymer ($f \ll 1$, $C_2 \ll C_3$), we face $q_0 \propto f l^{1/2}$.

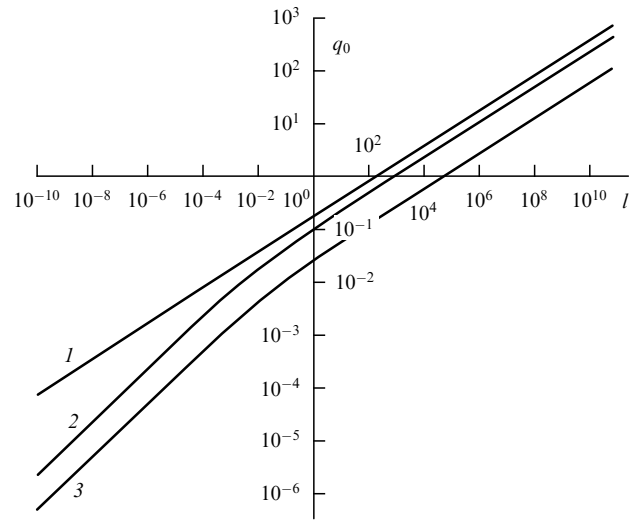


Figure 8. Macroscopic memory parameter q_0 vs. the value of the correlation length l (curves 1, 2, 3 correspond to $f = 0.5, 0.3, 0.1$).

The simultaneous solution of equations (4.48), (4.50), (4.51) yields the point χ_0 of ergodicity loss, whose position depending on the correlation length l is shown in Fig. 9 (thick lines). Observe that the nonzero value of the parameter χ_0 appears at some value of l above critical and, as l continues to increase, χ_0 reaches its maximum and begins to decline steadily. At moderate values of the correlation length l , the width of the ergodic region beneath the curve $\chi_0(l)$ decreases with increasing l . The condition $dg/d\chi = -\infty$ together with equalities (4.48), (4.50) leads to the equation

$$w + \mu^2(g_f + q) + \frac{\lambda^2}{2} (g_f + q)^2 = g_f^{-2} \quad (4.53)$$

which defines the value of the Flory–Huggins parameter at the vitrification point; below this point the microscopic

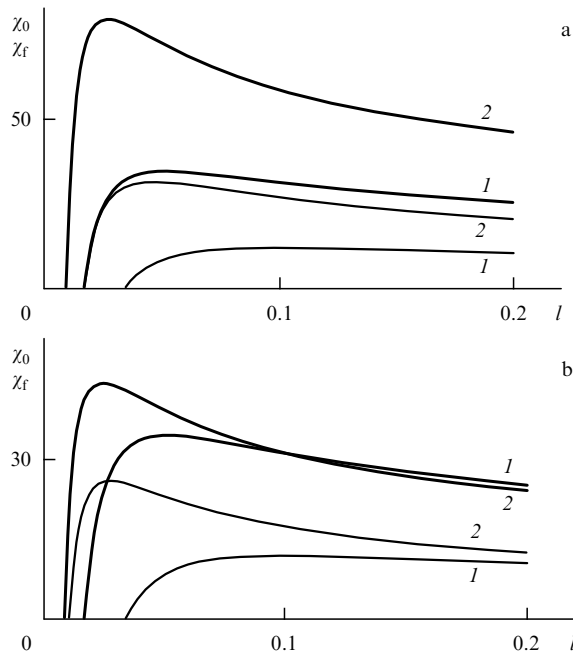


Figure 9. Characteristic values of the Flory–Huggins parameter at the point χ_0 of ergodicity loss (thick lines) and at the freezing point χ_f (thin lines) vs. the values of the correlation length l : (a) at $\sigma = 0$ and different compositions f (curves 1, 2 correspond to $f = 0.5, 0.3$); (b) at $f = 0.5$ and different values of the interreplica overlap parameter σ (curves 1, 2 correspond to $\sigma = 0, 1$).

susceptibility g is zero (Fig. 10). The corresponding dependence $\chi_f(l)$ on the correlation length is plotted in Fig. 9 (thin lines). Observe that curve $\chi_f(l)$ lies below the curve of ergodicity loss $\chi_0(l)$ and has the same shape. According to Fig. 9a, the parameters χ_0 and χ_f increase as we go away from the composition $f = 0.5$. More sophisticated behavior is associated with the increasing parameter σ of interreplica overlapping (see Fig. 9b): at small l , the increase in σ causes an increase in both χ_0 and χ_f , whereas at large values of the correlation length the parameter χ_0 decreases.

Figure 10 illustrates the macroscopic (g_0) and the microscopic (g) susceptibilities as functions of the Flory–Huggins parameter χ . Below the point χ_0 of ergodicity loss these susceptibilities, like the corresponding values q_0 , q of the memory parameter, are merged. At $\chi = \chi_f$, the curve $g(\chi)$ has a break, below which the susceptibility g assumes a zero value corresponding to the frozen state (see Section 2.8). Above the point χ_0 of ergodicity loss we have a constant value g_0 of the macroscopic susceptibility, and the steadily declining microscopic value g (the latter is found by solving equation (4.51) together with Eqn (4.48), in which the macroscopic parameters χ_0 , q_0 must be replaced with the microscopic parameters χ , q). According to Fig. 10a, as we go away from the composition $f = 0.5$, the values of susceptibilities at the points of ergodicity loss and freezing decrease, while the corresponding values of parameters χ_0 and χ_f increase. Figure 10b shows the curves $g(\chi)$, $g_0(\chi)$ for different values of the correlation length l ; as ought to be expected, the ergodic region narrows down as the correlation length increases. According to Fig. 10c, as the interreplica overlap parameter σ increases, the values of susceptibilities g and g_0 decrease, and hence this overlapping prevents the vitrification of a heteropolymer.

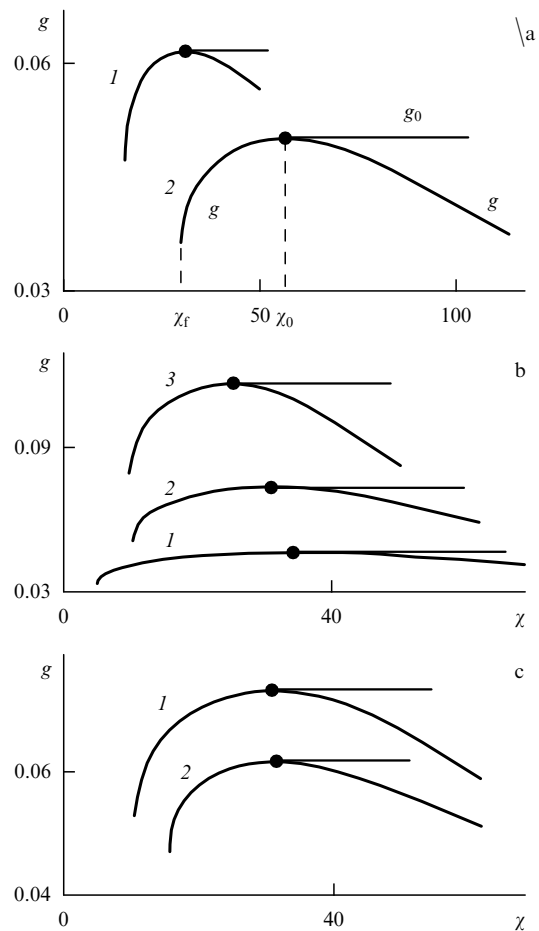


Figure 10. Microscopic (g) and macroscopic (g_0) susceptibilities vs. the Flory–Huggins parameter χ : (a) at $\sigma = 0$, $l = 0.1$ and different compositions f (curves 1, 2 correspond to $f = 0.5, 0.3$); (b) at $f = 0.5$, $\sigma = 0$ and different values of the correlation length l (curves 1, 2, 3 correspond to $l = 0.05, 0.1, 0.2$), and (c) at $f = 0.5$, $l = 0.1$ and different values of the interreplica overlap parameter σ (curves 1, 2 correspond to $\sigma = 0, 1$).

The effects of the thermodynamic parameter χ on the magnitude of the microscopic memory parameter q are illustrated in Fig. 11. The characteristic feature is the absence of memory below χ_f . A nonzero value of q appears at the freezing point χ_f , and as χ increases further the memory parameter steadily increases. The jump of parameter q at $\chi = \chi_f$ indicates that this transition is a first-order transition. Obviously, the physical cause of this jump is the contribution of fluctuations into the thermodynamic potential of the heteropolymer. According to Fig. 11a, as we go away from the composition $f = 0.5$, the curve $q(\chi)$ becomes more flat. The increase of the correlation length l , on the contrary, increases the rate of increase of the memory parameter (Fig. 11b). Finally, from Fig. 11c we see that the effects of the interreplica overlap parameter σ above and below the point of ergodicity loss are opposite.

The nonergodicity parameter Δ , shown in Fig. 12 as a function of χ , increases steadily as we recede from the point χ_0 . The deviation from the composition $f = 0.5$, the decrease of the correlation length l , and the increase of the interreplica overlap parameter σ all work to play down the effects of nonergodicity.

Figure 13 displays the phase diagram picturing the thermodynamic states of disordered heteropolymer at differ-

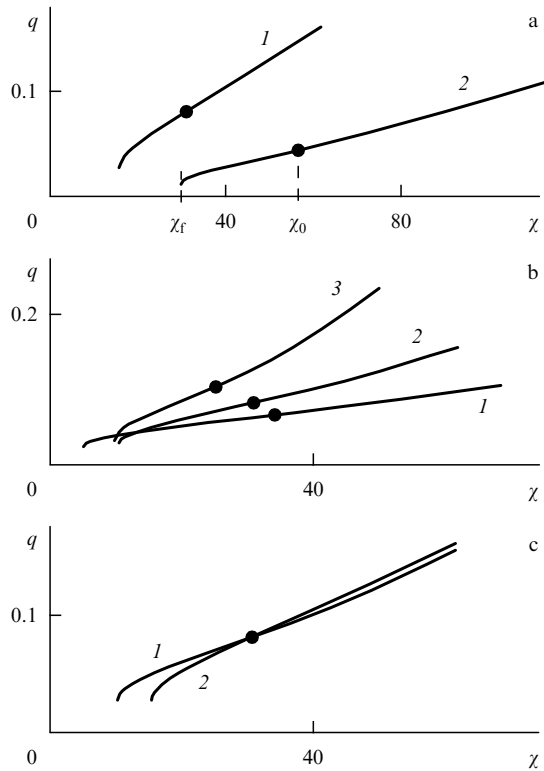


Figure 11. Microscopic memory parameter q vs. the Flory–Huggins parameter χ : (a) at $\sigma = 0$, $l = 0.1$ and different compositions f (curves 1, 2 correspond to $f = 0.5, 0.3$); (b) at $f = 0.5$, $\sigma = 0$ and different values of the correlation length l (curves 1, 2, 3 correspond to $l = 0.05, 0.1, 0.2$), and (c) at $f = 0.5$, $l = 0.1$ and different values of the interreplica overlap parameter σ (curves 1, 2 correspond to $\sigma = 0, 1$).

ent values of the Flory–Huggins parameter χ and composition f . We see that both at the vitrification point and at the point of ergodicity loss the curves $\chi_f(f)$, $\chi_0(f)$ are concave. The region of large values of χ , lying next to the composition $f = 0.5$, corresponds to the nonergodic nonfrozen state; as χ and $|f - 0.5|$ decrease, the system first goes into the ergodic state, and then vitrification takes place. Comparison between Figs 13a and 13b reveals that the increase of the correlation length l leads to the expansion of the frozen out and nonergodic phases. By contrast, from Figs 13a and 13c we see that overlapping between replicas gives rise to their narrowing.

5. Conclusions

Supersymmetry is one of the most beautiful and productive conceptions in contemporary physics, used for the description of the microworld (for introductory reading we recommend the reviews dealing with supersymmetry in quantum mechanics [85, 86], the theory of disordered metals [87], and the theory of superstrings [88–91]). Following the idea expressed in paper [56] and developed in work [57], we demonstrated earlier [58] how supersymmetry can be employed for the description of a macroscopic object that can be reduced to a fluctuating field (an example being the phase transition associated with the loss of symmetry). The present work is concerned with the study of stochastic systems whose phase space features a much more profound restructuring associated with the loss of ergodicity [92]. We apply to the field-

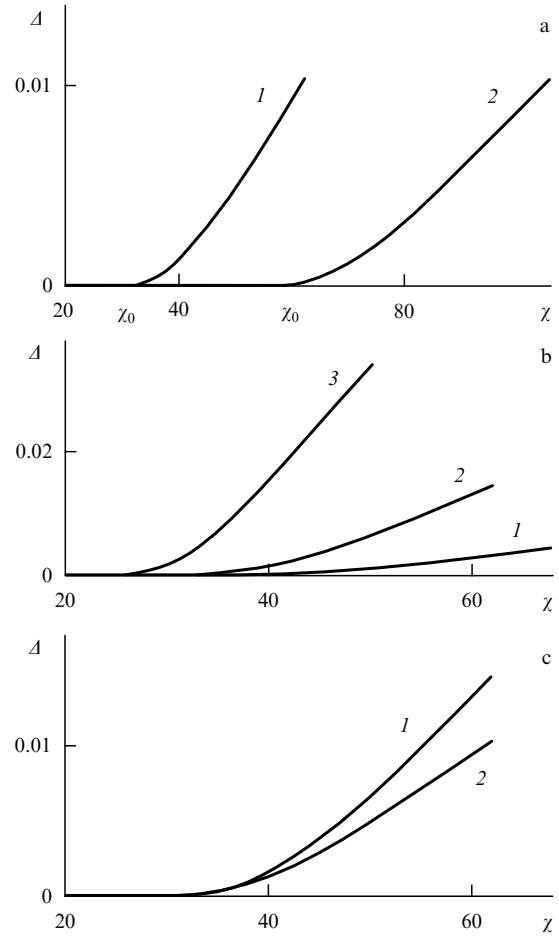


Figure 12. Nonergodicity parameter Δ vs. the Flory–Huggins parameter χ : (a) at $\sigma = 0$, $l = 0.1$ and different compositions f (curves 1, 2 correspond to $f = 0.5, 0.3$); (b) at $f = 0.5$, $\sigma = 0$ and different values of the correlation length l (curves 1, 2, 3 correspond to $l = 0.05, 0.1, 0.2$), and (c) at $f = 0.5$, $l = 0.1$ and different values of the interreplica overlap parameter σ (curves 1, 2 correspond to $\sigma = 0, 1$).

theoretical scheme based on the standard Martin–Siggia–Rose method [50], and on the idea of unifying the stochastic fields into the supersymmetric structure [56] (see also Ref. [51]).

Laying no claims whatsoever as to the originality of this method, we used a physical example that is interesting by itself to demonstrate that the use of supersymmetric field for the description of nonergodicity effects is as natural as the application to a complex field in the theory of phase transitions. From Section 2 we see that there are no associated fundamental difficulties as long as one has mastered the more sophisticated mathematical tools.

Unfortunately, the same cannot be said about the methodological problems that are associated both with the employment of the field-theoretical scheme and with the construction of the supersymmetric theory. As a matter of fact, a rare field-theoretical work avoids using the Hubbard–Stratonovich transformation, or a more intricate procedure by which unity is written down as the integral of a delta-function, which then is expanded in terms of the Fourier integral over the ghost field. As a result, one arrives at fictitious fields whose physical meaning gets no interpretation, and which are not even distinguished by special notation (‘capping the symbols’, etc.). The main purpose of this review

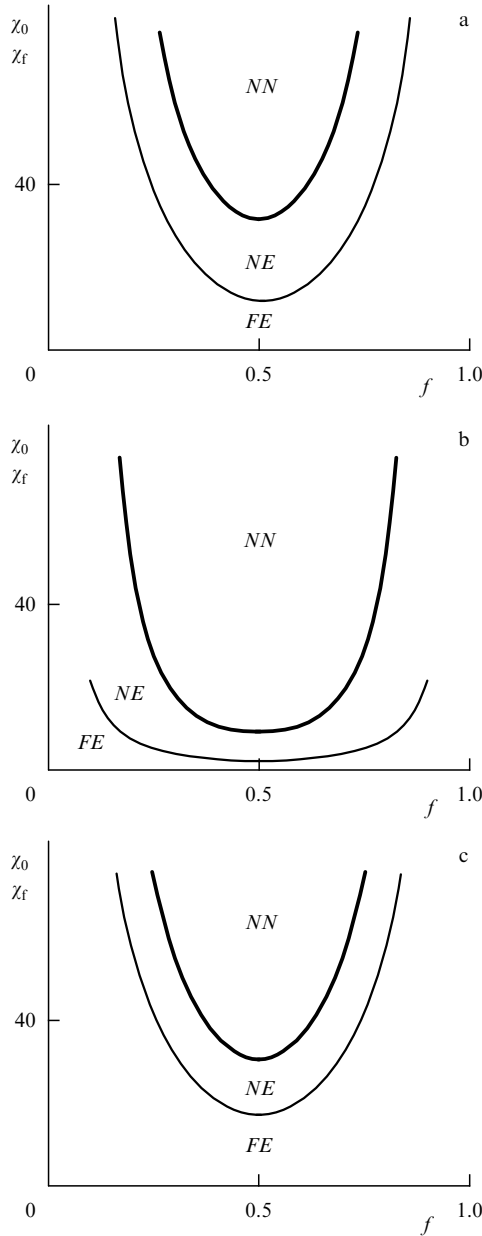


Figure 13. Phase diagram of a disordered heteropolymer: (a) at $\sigma = 0$, $D = 1$, $l = 0.1$; (b) at $\sigma = 0$, $D = 1$, $l = 5$, and (c) at $\sigma = 1$, $D = 1$, $l = 0.1$. The thick lines correspond to the loss of ergodicity, the thin lines conform to freezing, and the regions FE, NE, NN correspond to the frozen ergodic, frozen out ergodic and frozen out nonergodic phases, respectively.

is to break free from the situation when the clouds of ghosts obscure the physical meaning⁴. Of course, it is not possible to avoid the specific field procedures like the integral representations (2.8), (2.36) for the delta-function, and the Jacobian of transition from the stochastic component ζ of the conjugate field to the amplitude x of the hydrodynamic mode. But we then establish the physical meaning of the associated ghost field p and Grassmann fields $\psi, \bar{\psi}$.

⁴ In this connection we would like to recall the famous phrase of John Ziman: “A theoretical physicist is responsible for the purity of logical ways in construction of the theory, in the struggle against the flourishing phenomenological approach, with the hectic juggling with physical concepts, with the tautology of empty formalisms, with the hallucinations created by nonrealistic hypotheses” [93].

Our other task is related to overcoming the technical bottlenecks encountered in the construction of a supersymmetric scheme. These difficulties are due to the fact that, depending on the selection of the time origin, there are two possible variants of supersymmetric fields. Besides, a supersymmetric field can have either four or two components, in the latter case being not necessarily chiral. Given this variety of possibilities, we gave a comprehensive treatment in Section 2 to establish the linkage between different variants. This allowed us to pave the proper way for constructing the self-consistent supersymmetric scheme representing the stochastic system.

Finally, the practical purpose of this review consisted in the application of our supersymmetric scheme to a nontrivial object, the description of which with other methods seems to be either not feasible or highly contradictory. The ideal example, in our opinion, is the disordered heteropolymer. Indeed, while the random energy approximation only gives a qualitative picture of its behavior (see Section 1), the use of the replic method (Section 3) can lead to mutually exclusive results. Therefore, a basically new method of description of a disordered heteropolymer would be highly welcome from both theoretical and practical standpoints. Here, the main obstacle in the application of the concept of supersymmetry is the extreme complexity of the equation of motion of the polymer, which does not render itself for the construction of the generating functional. We avoided this difficulty by using the effective equation of motion, which describes the random alternation of monomers of different kinds when moving along the polymer chain.

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6. Appendices

6.1 Appendix A

Let us write out in the Lagrangian (2.10) of the Euclidean field theory the kinetic (κ) and the potential (π) energies:

$$L = \kappa + \pi, \quad (6.1)$$

$$\kappa = \varphi \dot{\eta} - \frac{1}{2} \varphi^2, \quad (6.2)$$

$$\pi = \frac{\partial V}{\partial \eta} \varphi. \quad (6.3)$$

To derive the kinetic energy (6.2) in the form (2.13), we need to find an operator D . In the general case it is represented in the following way

$$D = a + b \frac{\partial}{\partial \vartheta} + c \vartheta + d \vartheta \frac{\partial}{\partial \vartheta}, \quad (6.4)$$

where the coefficients a, b, c, d are functions of the derivative $\partial_t \equiv \partial/\partial t$. Substitution of expressions (2.11), (6.4) into (2.13) with due account for equalities (2.12) leads to the required expression (6.2) with the values

$$a = \partial_t, \quad b = -1, \quad c = 0, \quad d = -2\partial_t. \quad (6.5)$$

As a result, operator (6.4) takes on the form (2.14). It also satisfies the equality

$$D^2 = \partial_t^2. \quad (6.6)$$

Using definitions (2.11), (2.12), (2.14), it is easy to prove that the operator D is Hermitian.

The action of the infinitesimal operator

$$\delta \equiv \exp(\varepsilon D) - 1 \simeq \varepsilon D, \quad \varepsilon \rightarrow 0$$

on the quantities t and ϑ results in increments $\delta t = \varepsilon$, $\delta \vartheta = -\varepsilon$ which only differ in sign. In the treatment of the corresponding field variation $|\delta \phi_\varphi| = \varepsilon |D_\varphi| |\phi_\varphi|$, it is convenient to use the matrix representation of the nilpotent field (2.11) and the operator D :

$$|\phi_\varphi| = \begin{pmatrix} \eta \\ \varphi \end{pmatrix}, \quad |D_\varphi| = \begin{pmatrix} \partial_t & -1 \\ 0 & -\partial_t \end{pmatrix}, \quad \partial_t \equiv \frac{\partial}{\partial t}. \quad (6.7)$$

Hence it follows that the change in the order parameter is proportional to the difference between the rate of change of its magnitude and the amplitude of fluctuations, whereas the change of the latter is proportional to its rate taken with the opposite sign.

To reduce the nilpotent form (2.15) to the potential energy (6.3), we expand the thermodynamic potential at hand in powers of the term $\vartheta \varphi$ in Eqn (2.20):

$$\pi = \int \left[V(\eta) + \frac{\delta V}{\delta \eta} \varphi \vartheta \right] d\vartheta. \quad (6.8)$$

Here all terms of higher order vanish because of the nilpotency condition. Given the properties of equalities (2.12), the integration of Eqn (6.8) leads to the desired result (6.3).

The transition to the nilpotent field (2.30) is accomplished in a trivial way, so it will suffice to point to the differences from the case already considered. The infinitesimal transformation $\delta \simeq \varepsilon D$, where the generator D is given by equality (2.31), gives $\delta t = 0$, $\delta \vartheta = -\varepsilon$. The field variation $|\delta \phi_f| = \varepsilon |D_f| |\phi_f|$ is represented by matrices

$$|\phi_f| = \begin{pmatrix} \eta \\ -f \end{pmatrix}, \quad |D_f| = \begin{pmatrix} 0 & -1 \\ -\partial_t^2 & 0 \end{pmatrix}, \quad \partial_t \equiv \frac{\partial}{\partial t}. \quad (6.9)$$

Here the operator D_f exhibits the same property (6.6). It is easy to see that the Lagrangians (2.10), (2.25) are invariant with respect to transformations defined by generators D_φ , D_f if the infinitesimal parameter ε is purely imaginary, while the fields $\eta(\mathbf{r}, t)$, $\varphi(\mathbf{r}, t)$, $f(\mathbf{r}, t)$ are complex.

The matrices that provide the transition from field (6.9) to field (6.7) and back [see Eqns (2.32), (2.35)] look like

$$|\tau_{\pm}| = \begin{pmatrix} 1 & 0 \\ \pm \partial_t & 1 \end{pmatrix}. \quad (6.10)$$

Now let us consider the four-component supersymmetric fields (2.39), (2.52). As differentiated from Eqn (6.6), the corresponding pairs of operators (2.42), (2.53) obey the conditions

$$\begin{aligned} D^2 = \bar{D}^2 = 0, \quad \{\bar{D}, D\} = -2\partial_t, \quad [\bar{D}, D]^2 = (2\partial_t)^2, \\ \{D_\varphi, D_f\} = \{\bar{D}_\varphi, \bar{D}_f\} = 0, \quad \{\bar{D}_\varphi, D_f\} = -\partial_t, \\ \{\bar{D}_f, D_\varphi\} = -3\partial_t, \end{aligned} \quad (6.11)$$

where the braces and square brackets denote, respectively, anticommutators and commutators. For operators $\mathcal{D}^{(\pm)} \equiv \mathcal{D}(\pm t)$, $\bar{\mathcal{D}}^{(\pm)} \equiv \bar{\mathcal{D}}(\pm t)$ which correspond to different directions of time t , the generalized anticommuting relations acquire the form

$$\begin{aligned} \{\mathcal{D}^{(\pm)}, \mathcal{D}^{(\mp)}\} = \{\bar{\mathcal{D}}^{(\pm)}, \bar{\mathcal{D}}^{(\mp)}\} = \{\bar{\mathcal{D}}_f^{(\pm)}, \mathcal{D}_f^{(\mp)}\} = 0, \\ \{\bar{\mathcal{D}}^{(\pm)}, \mathcal{D}^{(\pm)}\} = -\{\bar{\mathcal{D}}_\varphi^{(\pm)}, \mathcal{D}_\varphi^{(\mp)}\} = \mp 2\partial_t; \\ \{\mathcal{D}_\varphi^{(\pm)}, \mathcal{D}_f^{(\pm)}\} = \{\bar{\mathcal{D}}_\varphi^{(\pm)}, \bar{\mathcal{D}}_f^{(\pm)}\} = 0, \quad \{\bar{\mathcal{D}}_\varphi^{(\pm)}, \mathcal{D}_f^{(\pm)}\} = \mp \partial_t, \\ \{\bar{\mathcal{D}}_f^{(\pm)}, \mathcal{D}_\varphi^{(\pm)}\} = \mp 3\partial_t; \\ \{\mathcal{D}_\varphi^{(\pm)}, \mathcal{D}_f^{(\mp)}\} = \{\bar{\mathcal{D}}_\varphi^{(\pm)}, \bar{\mathcal{D}}_f^{(\mp)}\} = 0, \\ \{\bar{\mathcal{D}}_\varphi^{(\pm)}, \mathcal{D}_f^{(\mp)}\} = \{\bar{\mathcal{D}}_f^{(\pm)}, \mathcal{D}_\varphi^{(\mp)}\} = \pm \partial_t. \end{aligned} \quad (6.12)$$

Relations (6.11), (6.12) are especially easily proved using a matrix representation similar to Eqns (6.7), (6.9):

$$\begin{aligned} |\Phi_\varphi| &= \begin{pmatrix} \eta \\ \psi \\ -\bar{\psi} \\ \varphi \end{pmatrix}, \\ |D_\varphi| &= \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -2\partial_t & 0 & 0 & 1 \\ 0 & 2\partial_t & 0 & 0 \end{pmatrix}, \quad |\bar{D}_\varphi| = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}; \end{aligned} \quad (6.13)$$

$$\begin{aligned} |\Phi_f| &= \begin{pmatrix} \eta \\ \psi \\ -\bar{\psi} \\ -f \end{pmatrix}, \\ |D_f| &= \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -\partial_t & 0 & 0 & 1 \\ 0 & \partial_t & 0 & 0 \end{pmatrix}, \quad |\bar{D}_f| = \begin{pmatrix} 0 & 0 & 1 & 0 \\ -\partial_t & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -\partial_t & 0 \end{pmatrix}. \end{aligned} \quad (6.14)$$

The transition matrices from field (6.14) to (6.13) are as follows [cf. Eqn (6.10)]

$$|T_{\pm}| = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \pm \partial_t & 0 & 0 & 1 \end{pmatrix}. \quad (6.15)$$

The action of infinitesimal operators $\delta \simeq \bar{\varepsilon} D$, $\bar{\delta} \simeq \bar{D} \varepsilon$ yields

$$\begin{aligned} \delta_\varphi \theta = 0, \quad \delta_\varphi \bar{\theta} = \bar{\varepsilon}, \quad \delta_\varphi t = -2\bar{\varepsilon} \theta, \\ \bar{\delta}_\varphi \theta = \varepsilon, \quad \bar{\delta}_\varphi \bar{\theta} = 0, \quad \bar{\delta}_\varphi t = 0; \\ \delta_f \theta = 0, \quad \delta_f \bar{\theta} = \bar{\varepsilon}, \quad \delta_f t = -\bar{\varepsilon} \theta, \\ \bar{\delta}_f \theta = \varepsilon, \quad \bar{\delta}_f \bar{\theta} = 0, \quad \bar{\delta}_f t = -\bar{\varepsilon} \varepsilon; \\ |\delta \Phi_\varphi| = \bar{\varepsilon} |D_\varphi| |\Phi_\varphi|, \quad |\bar{\delta} \Phi_\varphi| = |\bar{D}_\varphi| |\Phi_\varphi| \varepsilon; \\ |\delta \Phi_f| = \bar{\varepsilon} |D_f| |\Phi_f|, \quad |\bar{\delta} \Phi_f| = |\bar{D}_f| |\Phi_f| \varepsilon. \end{aligned} \quad (6.16)$$

By analogy with Eqn (6.8), for field (2.39) we have

$$\int V(\Phi_\varphi) d^2\theta = \frac{\delta V}{\delta\eta} \varphi - \bar{\psi} \frac{\delta^2 V}{\delta\eta^2} \psi. \quad (6.17)$$

Upon transition to field (2.52), in place of φ we observe $-f$.

6.2 Appendix B

Following the standard field-theoretical scheme [52], we split the four-component supersymmetric field (2.52) into a pair of chiral Grassmann conjugate two-component parts Φ_\pm . They may be obtained from the original superfield Φ_f in the following way

$$\Phi_\pm = T_\pm \Phi_f; \quad T_\pm \equiv \exp(\pm\partial), \quad \partial \equiv \bar{\theta}\partial_t, \quad \partial_t \equiv \frac{\partial}{\partial t}. \quad (6.18)$$

Accordingly, the generators (2.53) become

$$\mathcal{D}_\pm = T_\pm \mathcal{D}_f T_\pm, \quad \bar{\mathcal{D}}_\pm = T_\pm \bar{\mathcal{D}}_f T_\mp. \quad (6.19)$$

Taking advantage of the Grassmann nature of the parameter ∂ in operator T_\pm , we rewrite Eqn (6.19) as

$$\mathcal{D}_\pm = \mathcal{D}_f \pm [\partial, \mathcal{D}_f], \quad \bar{\mathcal{D}}_\pm = \bar{\mathcal{D}}_f \pm [\partial, \bar{\mathcal{D}}_f], \quad (6.20)$$

where the brackets denote a commutator. In the explicit form, we have

$$\begin{aligned} \mathcal{D}_+ &= \frac{\partial}{\partial\theta} - 2\theta\partial_t, \quad \mathcal{D}_- = \frac{\partial}{\partial\bar{\theta}}; \\ \bar{\mathcal{D}}_+ &= \frac{\partial}{\partial\bar{\theta}}, \quad \bar{\mathcal{D}}_- = \frac{\partial}{\partial\theta} - 2\bar{\theta}\partial_t. \end{aligned} \quad (6.21)$$

It is easy to show that the operators \mathcal{D}_+ , $\bar{\mathcal{D}}_+$ coincide with the generators \mathcal{D}_φ , $\bar{\mathcal{D}}_\varphi$ expressed by equalities (2.42).

According to definition (2.52), the transformations (6.18) give

$$\Phi_\pm = \eta + \bar{\theta}\dot{\psi} + \bar{\psi}\theta \pm \bar{\theta}\theta(\dot{\eta} \mp f), \quad (6.22)$$

where the over-dot denotes the time derivative. Comparing Eqn (6.22) with definition (2.39), we come to the identity $\Phi_+ \equiv \Phi_\varphi$. Applying operators (6.21) to the field (6.22), we get

$$\begin{aligned} \mathcal{D}_\pm \Phi_\pm &= \psi - \theta(\dot{\eta} + f) + \underline{2\bar{\theta}\theta\dot{\psi}}, \\ -\bar{\mathcal{D}}_\mp \Phi_\mp &= \bar{\psi} + \bar{\theta}(\dot{\eta} - f) - \underline{2\bar{\theta}\theta\dot{\bar{\psi}}}, \end{aligned} \quad (6.23)$$

where the underlined terms correspond to the superscripts.

By definition, the chiral supersymmetric fields are defined by the gauge conditions [52]

$$\mathcal{D}_- \Phi_- = 0, \quad \bar{\mathcal{D}}_+ \Phi_+ = 0 \quad (6.24)$$

which, in accordance with Eqn (6.21), imply that Φ_- does not depend on $\bar{\theta}$, and Φ_+ does not depend on θ . On the other hand, according to Eqn (6.23), the choice of the gauge (6.24) leads to the conditions

$$\begin{aligned} \psi - \theta(f + \dot{\eta}) &= 0, \\ \bar{\psi} + \bar{\theta}(\dot{\eta} - f) &= 0 \end{aligned} \quad (6.25)$$

for the fields Φ_- and Φ_+ , respectively. Substituting (6.25) into (6.22), we arrive at the final equations for chiral fields

$$\begin{aligned} \phi_- &= \eta + \bar{\psi}\theta, \\ \phi_+ &= \eta + \bar{\theta}\psi. \end{aligned} \quad (6.26)$$

They give the irreducible representation of supersymmetric fields (2.39), (2.52) with the gauge (6.24). The component $\phi_+(t)$ corresponds to the positive direction of time t , and $\phi_-(t)$ to the negative direction [52].

6.3 Appendix C

Consider the invariant properties of the supersymmetric action

$$\begin{aligned} S &= \int [K(\Phi(z)) + V(\Phi(z))] dz, \\ K(\Phi) &= \frac{1}{2} (\bar{\mathcal{D}}\Phi)(\mathcal{D}\Phi), \quad z \equiv \{\mathbf{r}, t, \theta, \bar{\theta}\}, \end{aligned} \quad (6.27)$$

with respect to the transformations

$$\delta\Phi = \sum_\alpha \bar{\epsilon}_\alpha \mathcal{D}^{(\alpha)}\Phi, \quad \bar{\delta}\Phi = \sum_\alpha \bar{\mathcal{D}}^{(\alpha)}\Phi \epsilon_\alpha \quad (6.28)$$

determined by the supersymmetric generators $\mathcal{D}^{(\alpha)}$, $\bar{\mathcal{D}}^{(\alpha)}$. These transformations are the combinations of derivatives with respect to time t and Grassmann coordinates $\theta, \bar{\theta}$. According to Eqn (6.17), the potential energy in Eqn (6.27) is invariant because its kernel does not depend on the time t . Accurately to the total time derivative, the Grassmann conjugate virials of the kinetic energy

$$\delta K = \frac{1}{2} \bar{\mathcal{D}} \left(\sum_\alpha \bar{\epsilon}_\alpha \mathcal{D}^{(\alpha)}\Phi \right) (\mathcal{D}\Phi) + \frac{1}{2} (\bar{\mathcal{D}}\Phi) \mathcal{D} \left(\sum_\alpha \bar{\epsilon}_\alpha \mathcal{D}^{(\alpha)}\Phi \right), \quad (6.29)$$

$$\bar{\delta} K = \frac{1}{2} \bar{\mathcal{D}} \left(\sum_\alpha \bar{\mathcal{D}}^{(\alpha)}\Phi \epsilon_\alpha \right) (\mathcal{D}\Phi) + \frac{1}{2} (\bar{\mathcal{D}}\Phi) \mathcal{D} \left(\sum_\alpha \bar{\mathcal{D}}^{(\alpha)}\Phi \epsilon_\alpha \right)$$

are written in the form

$$\begin{aligned} \delta K &= \frac{1}{2} \sum_\alpha \bar{\epsilon}_\alpha \mathcal{D}^{(\alpha)} [(\bar{\mathcal{D}}\Phi)(\mathcal{D}\Phi)], \\ \bar{\delta} K &= \frac{1}{2} \sum_\alpha \bar{\mathcal{D}}^{(\alpha)} [(\bar{\mathcal{D}}\Phi)(\mathcal{D}\Phi)] \epsilon_\alpha \end{aligned} \quad (6.30)$$

if the anticommutators $\{\mathcal{D}, \mathcal{D}^{(\alpha)}\}$, $\{\bar{\mathcal{D}}, \mathcal{D}^{(\alpha)}\}$, $\{\mathcal{D}, \bar{\mathcal{D}}^{(\alpha)}\}$, $\{\bar{\mathcal{D}}, \bar{\mathcal{D}}^{(\alpha)}\}$ are zero or can be reduced to a time derivative. According to relations (6.11), (6.12), these conditions hold true for the original operators \mathcal{D} , $\bar{\mathcal{D}}$, for operators \mathcal{D}_\pm , $\bar{\mathcal{D}}_\pm$ transformed according to relations (6.19), and for operators $\mathcal{D}_\pm^{(\pm)}$, $\bar{\mathcal{D}}_\pm^{(\pm)}$ corresponding to the opposite time directions. As combinations of derivatives with respect to time t and Grassmann coordinates $\theta, \bar{\theta}$, these operators yield zero variation of action (6.27) when substituted into expressions (6.30).

Out of the relations mentioned above, nontrivial properties are displayed by the operators

$$\mathcal{D}_-^{(-)} = \frac{\partial}{\partial\bar{\theta}}, \quad \bar{\mathcal{D}}_-^{(-)} = \frac{\partial}{\partial\theta} + 2\bar{\theta} \frac{\partial}{\partial t} \quad (6.31)$$

and by their anticommutator $\{\bar{\mathcal{D}}_-^{(-)}, \mathcal{D}_-^{(-)}\} = 2\partial_t$ [see Eqn (6.12)]. They result from the double application of transformation T_- to the original generators $\mathcal{D}_\varphi, \bar{\mathcal{D}}_\varphi$ and correspond to the generators $\mathcal{D}_-, \bar{\mathcal{D}}_-$ with the reversed time direction. This explains the fundamental importance of generators $\mathcal{D}_-^{(-)} \equiv \mathcal{D}_-(-t), \bar{\mathcal{D}}_-^{(-)} \equiv \bar{\mathcal{D}}_-(-t)$ defined by equalities (6.31).

Using straightforward algebra, it is easy to show that conditions $\delta S = 0, \bar{\delta} S = 0$ lead to the Ward identities [51]

$$\sum_{i=1}^n \mathcal{D}_i^{(x)} \Gamma^{(n)}(\{z_i\}) = 0, \quad \sum_{i=1}^n \bar{\mathcal{D}}_i^{(x)} \Gamma^{(n)}(\{z_i\}) = 0 \quad (6.32)$$

for the supersymmetric n -point irreducible vertex $\Gamma^{(n)}$ of the supercorrelator $C(z_2, z_1)$ type, or the self-energy superfunction $\Sigma(z_2, z_1)$. At $\mathcal{D}^{(x)} \equiv \partial_t, \bar{\mathcal{D}}^{(x)} \equiv \bar{\mathcal{D}}_-^{(-)}$, conditions (6.32) imply that the supercorrelators can only depend on the differences $t_2 - t_1, \bar{\theta}_2 - \bar{\theta}_1$:

$$C_\varphi(z_2, z_1) = S(t_2 - t_1) + (\bar{\theta}_2 - \bar{\theta}_1) \times [G_+(t_2 - t_1)\theta_2 - G_-(t_2 - t_1)\theta_1], \quad (6.33)$$

where we have dropped for brevity the dependence on coordinates. According to the definition of superfield (2.39), we have

$$\begin{aligned} S(t_2 - t_1) &= \langle \eta(t_2) \eta(t_1) \rangle, \\ G_+(t_2 - t_1) &= \langle \varphi(t_2) \eta(t_1) \rangle \vartheta(t_1 - t_2) \\ &= \langle \bar{\psi}(t_2) \psi(t_1) \rangle \vartheta(t_1 - t_2), \\ G_-(t_2 - t_1) &= \langle \eta(t_2) \varphi(t_1) \rangle \vartheta(t_2 - t_1) \\ &= \langle \bar{\psi}(t_1) \psi(t_2) \rangle \vartheta(t_2 - t_1), \end{aligned} \quad (6.34)$$

where $\vartheta(t) = 1$ at $t > 0$, and $\vartheta(t) = 0$ at $t < 0$. According to the causality condition, the advanced Green function $G_+(t_2 - t_1)$ in front of $\bar{\theta}_1\theta_2$ vanishes at $t_1 < t_2$; on the other hand, the retarded function $G_-(t_2 - t_1)$ corresponding to the term $\bar{\theta}_2\theta_1$ vanishes at $t_1 > t_2$. The condition of symmetry, $C(z_1, z_2) = C(z_2, z_1)$, leads to relations $S(t_2 - t_1) = S(t_1 - t_2)$, $G_-(t_2 - t_1) = G_+(t_1 - t_2)$. Substitution of operator $\bar{\mathcal{D}}_-^{(-)}$ into the Ward identity (6.32) gives the equation

$$2\dot{S}(t) = G_+(t) - G_-(t) \quad (6.35)$$

which reduces to the fluctuation-dissipative theorem in the time-domain representation. Obviously, these arguments apply not only to the supercorrelator, but also to the self-energy superfunction whose components $\Sigma(t_2 - t_1), \Sigma_\pm(t_2 - t_1)$ correspond to $S(t_2 - t_1), G_\pm(t_2 - t_1)$.

The supersymmetric nature of relations (6.34) is manifested in that they link the correlators of the Bose components η, φ and Fermi components $\psi, \bar{\psi}$. Ward identities (6.32), used above, allowed these relations to be obtained as a trivial implication of the definition of supersymmetric field (2.39). However, these equations can also be obtained in an elementary way. Indeed, according to the definitions (2.23), (2.38), the Fermi correlator $\langle \bar{\psi}\psi \rangle$ is $(\delta^2 V / \delta \eta^2)^{-1}$. On the other hand, using the definition of susceptibility and equalities (2.24), (2.28), for the Bose correlator we have $\langle \eta\varphi \rangle = \langle \delta\eta / \delta\varphi \rangle = \langle (\delta\varphi / \delta\eta)^{-1} \rangle = (\delta^2 V / \delta \eta^2)^{-1}$, which gives us the result wanted.

Obviously, for the transition to the correlators of a two-component nilpotent field (2.11), we need to replace the

multipliers $(\bar{\theta}_2 - \bar{\theta}_1)\theta_2, (\bar{\theta}_2 - \bar{\theta}_1)\theta_1$ in Eqn (6.33) with the nilpotent coordinates $\vartheta_2, -\vartheta_1$, and drop out the term $\bar{\vartheta}_2\vartheta_1$.

The supersymmetric correlator

$$C_f(z_2, z_1) = T_-(z_2)T_-(z_1)C_\varphi(z_2, z_1)$$

corresponding to the supefields (2.30), (2.52) is represented as

$$C_f(z_2, z_1) = S + \bar{\theta}_2\theta_2 m_+ + \bar{\theta}_1\theta_1 m_- - \bar{\theta}_2\theta_1 G_- - \bar{\theta}_1\theta_2 G_+, \quad (6.36)$$

where we have dropped out the arguments $t_2 - t_1$ in the terms S, m_\pm, G_\pm and, with due account for expression (2.24), introduced the functions [cf. Eqn (6.34)]

$$\begin{aligned} m_+(t) &= \langle \eta(-t) \rangle \vartheta(-t) f_{\text{ext}}, \\ m_-(t) &= \langle \eta(t) \rangle \vartheta(t) f_{\text{ext}}, \quad f_{\text{ext}} \equiv -f, \end{aligned} \quad (6.37)$$

which define the linkage between the mean order parameter $\langle \eta(t) \rangle$ and the external force $f_{\text{ext}} \equiv -f$ (it is assumed that the latter is switched on at $t = 0$ and keeps its magnitude). Correlators (6.37) are linked with the Green functions by the equality

$$G_\pm(t) = m_\pm(t) \pm \dot{S}(t) \quad (6.38)$$

and comply with the symmetry condition $m_+(-t) = m_-(t)$.

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