Equilibrium Ensemble Approach to Disordered Systems I: General Theory, Exact Results

Reimer Kühn*
Institut für Theoretische Physik, Universität Heidelberg
Philosophenweg 19, 69120 Heidelberg, Germany
e–mail: kuehn@hybrid.tphys.uni-heidelberg.de

May 1995

Abstract An outline of Morita's equilibrium ensemble approach to disordered systems is given, and hitherto unnoticed relations to other, more conventional approaches in the theory of disordered systems are pointed out. It is demonstrated to constitute a generalization of the idea of grand ensembles and to be intimately related also to conventional low–concentration expansions as well as to perturbation expansions about ordered reference systems. Moreover, we draw attention to the variational content of the equilibrium ensemble formulation. A number of exact results are presented, among them general solutions for site– and bond– diluted systems in one dimension, both for uncorrelated, and for correlated disorder.

1 Introduction

The present contribution is concerned with the statistical mechanics of systems with quenched randomnes. According to a seminal paper by Brout [1], the relevant thermodynamic potential for the description of such systems is the average of the free energy of the system over the distribution $q(\kappa)$ describing the disorder configurations κ,

$$f_q = -(\beta N)^{-1} \left\langle \ln Z_N(\kappa) \right\rangle_q \ . \tag{1}$$

Here N denotes the system size, and $Z_N(\kappa)$ is the partition function of a system of size N at fixed disorder configuration κ.

The evaluation of the quenched free energy (1) is difficult for at least two reasons. First, in virtually all configurations κ contributing to the average, the system is not translationally invariant — a circumstance invalidating all conventional calculational tools relying on such invariance. Moreover, averaging the logarithm of the partition function usually precludes any useful factorization of the averaging process even in situations where such factorization is possible when considering the average of $Z_N(\kappa)$ itself.

*Supported by a Heisenberg fellowship

For the reasons just outlined only few exactly solved models of systems with quenched disorder are known. Where solutions of such models *have* been obtained, success has as a rule been due to simplifying features, such as one–dimensionality of the models (see [2] for a recent overwiew) or of the disorder type [3], analytic structures available in spherical models [4] or infinite dimensionality where mean–field approximations are exact (see, e.g. [5]).

Discomforting to a perhaps even greater degree is the fact that conventional asymptotic methods for the study of phase transitions and critical phenomena, such as series expansions, renormalization group or Monte–Carlo calculations, have in several cases procuced conflicting and sometimes even spurious results, when applied to disordered systems. This being so, alternative approaches are clearly welcome.

The present contribution is devoted to one such alternative, which is at the same time venerable, *not* well known and still, we believe, promising. The method is originally due to Morita [6]. The main idea is to treat the configurational degrees of freedom κ on the same footing as the dynamical variables proper, and to supplement the Hamiltonian of the disordered system by a disorder potential $\phi(\kappa)$ which is determined such that configuration averaging as implied by (1) becomes part of the Gibbs average in an enlarged phase space. By this device, it is hoped, the full machinery of equilibrium statistical physics is made available for the study of systems with quenched randomness. The idea of an equivalent equilibrium ensemble naturally lends itself to the formulation of systematic approximative schemes. The perhaps most natural was already suggested by Morita [6]; it starts out from the so–called annealed approximation, which is then improved by imposing an increasing number of constraints on the thermal motion of the configurational degrees of freedom. Thus, as pointed out by Falk [7], annealed approximations, such as employed by Thorpe and Beeman [8] to determine phase boundaries in bond–disordered 2–D Ising models, constitute just the first step wihtin Morita's restricted annealing scheme.

The Morita approach is natural enough to have been used, reconsidered, or rediscovered several times. Thorpe [9] applied essentially this idea to improve upon annealed phase boundaries obtained earlier [8], a topic taken up again somewhat later by George et al. [10], who fell on virtually the same set of ideas, arguing from a somewhat different point of view, though. Restricted annealing has been discussed in connection with spin–glasses by Toulouse and Vannimenus [11], who also drew attention to formal similarities with lattice gauge theories.

Explicit reference to Morita's original paper is made in [12] – [17]. Sobotta and Wagner [12], restricting themselves to bimodal disorder (see below), streamlined the formal presentation of the approach, and applied it in conjunction with the renormalization group and the ε–expansion to study spin–diluted ferromagnets near dimension 4 [13]. Huber [14] discusses the *thermodynamic* content of the Morita scheme and derives a normalization condition for the disorder potential $\phi(\kappa)$ from thermodynamic consistency–considerations. In [15], [17], Kühn combines restricted annealing with the phenomenological renormalization group method to study the critical behaviour of the 2–D spin–diluted Ising model, while Kühn *et al.* [16] apply constrained annealing to provide an exact solution of van Hemmen's spin–glass model [18].

Somewhat earlier restricted annealing was rediscovered by Schwartz [19] and put for-

ward in the debate about the lower critical dimension of the random field Ising model (RFIM), incidentally producing results compatible with the more recent rigurous proof of stability of ferromagnetism in the three dimensional RFIM [20]. The most recent rediscovery of the method is due to Serva and Paladin [21], who used it to study the mean–field version of the RFIM, which is actually somewhat simpler that the model considered in [16], and who produced approximate numerical solutions of the RFIM in 1–D.

The purpose of the present paper is to give an outline of the formal and systematic aspects of Morita's equilibrium ensemble approach to disordered systems. Sec. 2 summarizes for future reference the general theory, and formulates constrained annealing as the canonical approximative scheme that derives from it. In this context it is emphasized that the equilibrium ensemble approach is nothing but a generalization of the grand ensemble idea [17]. Alternatively, it can be looked upon as a method for obtaining variational lower bounds for quenched free energies. In Sec. 3 we specialize to bimodal bond– or site–disorder, and point out a connection to a different well established set of ideas, namely the relation to conventional low–concentration expansions and to perturbation expansions about homogeneous reference systems. For systems with bond– or site–dilution additional information about the exact disorder potential $\phi(\kappa)$ can be obtained which is used among other things to provide exact general solutions to the 1–D case. The equilibrium ensemble approach is well suited to study systems with correlated quenched disorder. Sec. 4 develops this point to some extent. In Sec. 5 we briefly indicate a range of alternative possibilities to formulate truncation and approximation schemes within the general approach, and we end with an outlook and concluding remarks. Constrained annealing as a method to study the thermodynamics and critical behaviour of disordered Ising models will be taken up in greater detail in an accompanying paper [22], to be referred to as II in what follows. A short version collecting the main results of that study has appeared elsewhere [17]. The contents of Sec. 2 are not entirely new. Large parts of the general theory, in particular Secs. 2.1–2.4, have more or less explicitly appeared before — notably in [6], [12]. What we can perhaps claim originality for, is for pointing out heretofore unnoticed connections to other sets of ideas (to grand canonical ensembles, to variational bounding of free energies, and to low–concentration and perturbation expansions) as well as for the collection of exact results presented in Secs. 3 and 4.

2 General Theory

2.1 Equilibrium Ensemble Approach to Disordered Systems

In order to avoid the complications associated with the evaluation of quenched averages, Morita [6] suggested to introduce an equivalent ensemle in which configurational averaging becomes part of the thermal averaging procedure in an enlarged phase space that is defined over both, the configurational degrees of freedom κ, and the dynamical variables proper. This is achieved by introducing a "ficticious" disorder potential $\phi(\kappa)$ which is added to the system Hamiltonian

$$\mathcal{H}(\sigma|\kappa) \to \mathcal{H}^{\phi}(\sigma,\kappa) = \mathcal{H}(\sigma|\kappa) + \phi(\kappa) \tag{2}$$

and chosen such that the system described by $\mathcal{H}^\phi$ will have thermodynamic equilibrium properties identical to the nonequilibrium properties of the quenched system.[1] In a first step, therefore, it is required that the Gibbs-Boltzmann distribution generated by $\mathcal{H}^\phi$

$$p^\phi(\sigma,\kappa) = \frac{1}{Z^\phi}\exp[-\beta\mathcal{H}^\phi(\sigma,\kappa)] \tag{3}$$

be equal to the non–equilibrium distribution

$$p_q(\sigma,\kappa) = \frac{q(\kappa)}{Z(\kappa)}\exp[-\beta\mathcal{H}(\sigma|\kappa)] \tag{4}$$

describing the joint statistics of configurational and dynamical degrees of freedom in an ensemble of quenched systems. That is, one demands

$$p^\phi(\sigma,\kappa) = p_q(\sigma,\kappa) \tag{5}$$

for all (σ,κ). This equation can be solved for ϕ to yield

$$\beta\phi(\kappa) = -\ln[q(\kappa)/Z(\kappa)] - \ln Z^\phi \ . \tag{6}$$

We shall in what follows refer to (6) as to the Morita equation. It expresses the fact that an equivalent equilibrium ensemble exists. As long as one is interested only in its probabilistic content, Eqs. (2), (3) and (6) are all one needs in principle. In practice, of course, not much has been gained so far. The translation of the problem of configuration averaging in systems with quenched randomness into the language of an equivalent equilibrium ensemble is *purely formal*. It does not so far help to circumvent any of the difficulties for which it was invented to begin with. To use the idea in practice, one has to find a *representation* for the potential $\phi(\kappa)$, which is adapted to the given disorder problem, and which can be the starting point for the construction of systematic approximation schemes.

Before turning to this topic in the following subsection, let us address the thermodynamic content of the equivalent equilibrium ensemble. It was pointed out by Huber [14], that due to the invariance of (6) under the transformation

$$\phi(\kappa) \ \rightarrow \ \phi(\kappa) + \phi_0 \ , \tag{7}$$

$$Z^\phi \ \rightarrow \ Z^\phi \exp[-\beta\phi_0] \ , \tag{8}$$

the disorder potential ϕ and thus the equilibrium ensemle's partition function Z^ϕ are specified only up to arbitrary constants ϕ_0 (constant in the sense that they do not depend on the disorder configuration κ) , which may, however, still depend on temperature, external fields, coupling constants, impurity concentration and so on. For the probabilistic content of the theory, this need not be a point of concern. If, however, one also demands that

$$F^\phi = -\beta^{-1}\log Z^\phi \tag{9}$$

be identified with the free energy of the equivalent equlibrium ensemble, a normalization is clearly needed. It was demonstrated by Huber [14] that thermodynamic consistency —

[1] Here and in what follows, we suppress indices signifying the system–size dependences of various quantities, in order to simplify notation.

equality of probabilistic and thermodynamic definitions of internal energy, entropy, and other thermodynamic functions involving derivatives of F^ϕ up to first order in temperature and fields — requires the configuration average of ϕ to vanish,

$$\langle \phi(\kappa) \rangle_q = \sum_\kappa q(\kappa)\phi(\kappa) = 0 \ . \tag{10}$$

Indeed, with this condition it follows from (6) that

$$-\beta F^\phi = \ln Z^\phi = \langle \ln Z(\kappa) \rangle_q - \langle \ln q(\kappa) \rangle_q \ , \tag{11}$$

so that F^ϕ gives the quenched free energy plus a contribution which is easily identified with an entropy of mixing,

$$k_{\rm B}^{-1} S_0 = - \langle \ln q(\kappa) \rangle_q = - \sum_\kappa q(\kappa) \ln q(\kappa) \ . \tag{12}$$

Since this extra contribution is independent of temperature and external fields, it is irrelevant for thermodynamics. With the normalization condition imposed, the disorder potential ϕ reads

$$\beta\phi(\kappa) = - \left[\ln \frac{q(\kappa)}{Z(\kappa)} - \left\langle \ln \frac{q(\kappa)}{Z(\kappa)} \right\rangle_q \right] \ , \tag{13}$$

which shows that a full specification of ϕ requires the computation of the quenched free energy — precicely the quantity the computation of which the equilibrium ensemble approach was invented to facilitate, not to speak of the difficulties of solving or analysing models with a contribution to the potential energy as complicated as (13). On the other hand Eq. (13) shows that, having computed a properly normalized $\phi(\kappa)$, it suffices to evaluate it for a simple homogeneous configuration κ to obtain essentially the Brout free energy.

2.2 Constrained Entropy Maximization

In order to introduce an alternative and more explicit representation of the disorder potential ϕ, which can serve as a starting point for systematic approximation schemes, it is advantageous to recall Mazo's [23] information-theoretic justification of Brout's averaging prescripton.

The distribution $p_q(\sigma, \kappa)$ which reproduces Brout's averaging prescription for the free energy can according to Mazo be derived from Jaynes' information–theoretic approach to statistical mechanics [24]. That is, it is given as the unique distribution which maximizes the entropy functional

$$S[p] = -k_{\rm B} \sum_{\sigma,\kappa} p(\sigma,\kappa) \ln p(\sigma,\kappa) \tag{14}$$

under the constraints

$$\langle \mathcal{H}(\sigma|\kappa) \rangle_p \quad = \textstyle\sum_{\sigma,\kappa} p(\sigma,\kappa) \mathcal{H}(\sigma|\kappa) \quad = E \tag{15}$$

$$\langle \delta(\kappa - \kappa') \rangle_p \quad = \textstyle\sum_{\sigma,\kappa} p(\sigma,\kappa) \delta(\kappa - \kappa') \quad = q(\kappa') \ , \qquad \forall\ \kappa' \ . \tag{16}$$

Eq. (15) fixes the average energy of the system, while (16) demands that the search for maximizing distributions is restricted among those compatible with the a–priori distribution $q(\kappa)$ characterizing the disorder. Introducing Lagrangian multipliers $-k_{\rm B}\beta$ and $k_{\rm B}(\lambda(\kappa)+1)$ to enforce the constraints, one obtains $p_q(\sigma,\kappa)$ defined by

$$S[p_q] = \max_p \Big\{ S[p];\ \langle \mathcal{H}(\sigma|\kappa)\rangle_p = E \text{ and } \langle \delta(\kappa-\kappa')\rangle_p = q(\kappa')\ \forall\ \kappa' \Big\} \tag{17}$$

in the form

$$p_q(\sigma,\kappa) = \exp[-\beta\mathcal{H}(\sigma,\kappa) + \lambda(\kappa)] \ . \tag{18}$$

To satisfy (16), one needs

$$\exp[\lambda(\kappa)] = \frac{q(\kappa)}{Z(\kappa)} \ , \tag{19}$$

where $Z(\kappa)$ is the partition sum at fixed disorder configuration κ, so that (18) does, indeed, agree with (4), and we have seen in the previous subsection that it can be interpreted as an equilibrium distribution p^ϕ in an enlarged phase space.

2.3 Alternative Formulation of Constrained Entropy Maximization (Bimodal Disorder)

The alternative representation of ϕ announced above is obtained by replacing the constraints (16) in the above entropy–maximization procedure by an equivalent set of constraints, namely by the requirement that the search for maximizing distributions is restricted to those which reproduce the *complete set of moments* of $q(\kappa)$.

To be specific, and to keep notation and formulae as trasparent as possible, let us first consider the case of systems with *bimodal* site (bond) disorder, in which a random variable associated with each site (bond) of the lattice can only take two values. We shall explain the necessary modifications to treat more general types of randomnes in Sec. 2.5 below. Bimodal disorder is conveniently described in terms of site (bond) *occupation numbers* $k_a = k_a(\kappa)$ which take the values 0 or 1, if on the a–th site (bond) one or the other of the two possible realizations of the disorder is attained in the configuration κ. The set of moments of $q(\kappa)$ is given by the expectation under $q(\kappa)$ of all possible products of occupation numbers k_a,

$$f_\omega = \left\langle \prod_{a\in\omega} k_a(\kappa) \right\rangle_q \ , \qquad \omega \subseteq \Lambda \ , \tag{20}$$

where ω ranges through all subsets of the set Λ of sites (bonds) of the lattice, including the empty set. It is useful introduce occupation numbers for the sets ω through

$$k_\omega(\kappa) = \prod_{a\in\omega} k_a(\kappa) \ , \tag{21}$$

with $k_\emptyset(\kappa) \equiv 1$, and to identify κ with the set of vertices (bonds) for which $k_a = 1$, that is, $\kappa = \{k_a; a\in\Lambda\} \equiv \{a\in\Lambda; k_a = 1\}$. This allows to write

$$f_\omega = \langle k_\omega(\kappa)\rangle_q = \sum_{\substack{\kappa \\ \kappa \supseteq \omega}} q(\kappa) \ . \tag{22}$$

In the present case, the equivalence of the system of moments f_ω and the distribution $q(\kappa)$ follows directly from the invertibility of (22),

$$q(\kappa) = \sum_{\substack{\omega \\ \omega \supseteq \kappa}} (-1)^{|\omega|-|\kappa|} f_\omega \ , \tag{23}$$

where $|\omega|$ and $|\kappa|$ denote the size of the sets ω and κ, respectively. The set of moments can be used to reformulate the constrained entropy maximization, by replacing (16) with

$$\langle k_\omega(\kappa) \rangle_q = \sum_{\sigma,\kappa} p(\sigma,\kappa) k_\omega(\kappa) = f_\omega \ , \qquad \omega \subseteq \Lambda \ . \tag{24}$$

Since (16) and (24) are *equivalent* sets of constraints, one can alternatively obtain $p_q(\sigma,\kappa)$ through

$$S[p_q] = \max_p \Big\{ S[p];\ \langle \mathcal{H}(\sigma|\kappa) \rangle_p = E \text{ and } \langle k_\omega(\kappa) \rangle_p = f_\omega \ ,\ \omega \subseteq \Lambda \Big\} \ . \tag{25}$$

Denoting the Lagrangian multipliers that enforce (15) and (24) by $-k_{\rm B}\beta$ and $k_{\rm B}(\lambda_\omega + \delta_{\omega,\emptyset})$, one obtains the maximizing distribution p_q in the form

$$p_q(\sigma,\kappa) = \exp\Big[-\beta \mathcal{H}(\sigma|\kappa) + \sum_{\omega \subseteq \Lambda} \lambda_\omega k_\omega(\kappa) \Big] \ . \tag{26}$$

Writing

$$\lambda_\emptyset = -\ln \mathcal{Z}, \tag{27}$$

one gets

$$p_q(\sigma,\kappa) = \frac{1}{\mathcal{Z}} \exp\Big[-\beta \mathcal{H}(\sigma|\kappa) + \sum_{\emptyset \neq \omega \subseteq \Lambda} \lambda_\omega k_\omega(\kappa) \Big] \ , \tag{28}$$

where the λ_ω, $\omega \neq \emptyset$, must be determined such that p_q satisfies (24) for the set of moments of the distribution $q(\kappa)$ describing the disorder. Thus, an explicit representation of $\phi(\kappa)$ in terms of weighted sums of products of occupation numbers has been obtained. The representation (28) of the distribution $p_q(\sigma,\kappa)$ has been advanced already by Morita [6], in a more transparent way, though, by Sobotta and Wagner [12].

Note that $\mathcal{Z}$ has the formal appearance of a generalized grand partition sum, with generalized chemical potentials given by $\mu_\omega = \beta^{-1}\lambda_\omega$. The corresponding generalized grand potential is

$$\Omega = -\beta^{-1} \ln \mathcal{Z} \ , \tag{29}$$

and one has

$$f_\omega = \langle k_\omega \rangle = -\frac{\partial \Omega}{\partial \mu_\omega} \ . \tag{30}$$

Returning to the general considerations of the previous subsection, we realize that in the form in which the disorder potential appears in (28),

$$\beta\phi(\kappa) = -\sum_{\emptyset \neq \omega \subseteq \Lambda} \lambda_\omega k_\omega(\kappa) \ , \tag{31}$$

it does *not* satisfy the normalization condition (10). To enforce it, one changes ϕ according to

$$\beta\phi(\kappa) \to -\sum_{\emptyset\neq\omega\subseteq\Lambda} \lambda_\omega (k_\omega(\kappa) - f_\omega) \ . \tag{32}$$

On the level of thermodynamic potentials, this change amounts to a Legendre–transform from the generalized grand potential to the corresponding free energy,

$$\Omega \to F^\phi = \Omega + \sum_{\emptyset\neq\omega\subseteq\Lambda} \mu_\omega f_\omega = \Omega - \sum_{\emptyset\neq\omega\subseteq\Lambda} \mu_\omega \frac{\partial\Omega}{\partial\mu_\omega} \ . \tag{33}$$

Finally, using (27), (33) and the fact that $f_\emptyset = 1$ due to the normalization of $p^\phi = p_q$, one obtains an intriguingly simple representation of the equivalent ensemble's free energy, viz.

$$-\beta F^\phi = \ln Z^\phi = -\sum_{\omega\subseteq\Lambda} \lambda_\omega f_\omega \ . \tag{34}$$

Note that determining the λ_ω such as to make p^ϕ satisfy the constraints defining the disorder distribution is tantamount to *minimizing* $\ln Z^\phi$ with respect to the λ_ω. Phrased differently, it means minimizing $\ln Z^\phi$ over a space of functions $\phi(\kappa)$ which are of the form (32).

2.4 A Canonical Approximative Scheme: Constrained Annealing (Bimodal Disorder)

The simplicity of (34) is, of course, purely formal and hence deceptive. Nevertheless, something non–trivial has been gained, namely an *explicit* representation for the disorder potential ϕ, together with a method to compute it that immediately lends itself to the formulation of a systematic scheme of approximations. This scheme consists of replacing the full set (24) of constraints by a subset which requires the maximizing distributions to reproduce only a given subset of the full set of moments of $q(\kappa)$.

Formally, let $\mathcal{Q}$ be a subset of the powerset $\mathcal{P}(\Lambda)$ of the vertices or bonds of the lattice, and define $p^\mathcal{Q}$ as the unique distribution that maximizes the entropy functional (14) under the constraints

$$\langle \mathcal{H}(\sigma|\kappa)\rangle_p \quad = \textstyle\sum_{\sigma,\kappa} p(\sigma,\kappa)\mathcal{H}(\sigma|\kappa) \quad = E \tag{35}$$

$$\langle k_\omega(\kappa)\rangle_p \quad = \textstyle\sum_{\sigma,\kappa} p(\sigma,\kappa)k_\omega(\kappa) \quad = f_\omega \ , \quad \omega\in\mathcal{Q} \ , \tag{36}$$

that is,

$$S[p^\mathcal{Q}] = \max_p \Big\{ S[p];\ \langle \mathcal{H}(\sigma|\kappa)\rangle_p = E \text{ and } \langle k_\omega(\kappa)\rangle_p = f_\omega \ ,\ \omega\in\mathcal{Q} \Big\} \ . \tag{37}$$

Introducing Lagrangian multipliers $-k_\mathrm{B}\beta$ and $k_\mathrm{B}(\lambda^\mathcal{Q}_\omega + \delta_{\omega,\emptyset})$, $\omega\in\mathcal{Q}$, one obtains the maximizing distribution $p^\mathcal{Q}$ in the form

$$p^\mathcal{Q}(\sigma,\kappa) = \exp\Big[-\beta\mathcal{H}(\sigma|\kappa) + \sum_{\omega\in\mathcal{Q}} \lambda^\mathcal{Q}_\omega k_\omega(\kappa)\Big] \ . \tag{38}$$

Writing

$$\lambda_{\emptyset}^{\mathcal{Q}} = -\ln \mathcal{Z}^{\mathcal{Q}} \ , \tag{39}$$

one observes that this takes the form of a generalized grand–canonical distribution

$$p^{\mathcal{Q}}(\sigma,\kappa) = \frac{1}{\mathcal{Z}^{\mathcal{Q}}} \exp\Big[-\beta\mathcal{H}(\sigma|\kappa) + \sum_{\emptyset\neq\omega\in\mathcal{Q}} \lambda_{\omega}^{\mathcal{Q}} k_{\omega}(\kappa)\Big] \ , \tag{40}$$

where one has to determine the $\lambda_{\omega}^{\mathcal{Q}} = \beta\mu_{\omega}^{\mathcal{Q}}$ such as to satisfy the constraints (36). In order to obtain the free energy corresponding to the $\mathcal{Q}$–approximation, one has to enforce the zero–mean-potential condition (10) by changing $\phi^{\mathcal{Q}}$ according to

$$\beta\phi^{\mathcal{Q}}(\kappa) \to -\sum_{\emptyset\neq\omega\in\mathcal{Q}} \lambda_{\omega}^{\mathcal{Q}}(k_{\omega}(\kappa) - f_w) \ . \tag{41}$$

As above, this amounts to a Legendre transformation from the generalized grand potential

$$\Omega^{\mathcal{Q}} = -\beta^{-1}\ln \mathcal{Z}^{\mathcal{Q}} \tag{42}$$

to the corresponding free energy

$$\Omega^{\mathcal{Q}} \to F^{\mathcal{Q}} = \Omega^{\mathcal{Q}} + \sum_{\emptyset\neq\omega\in\mathcal{Q}} \mu_{\omega}^{\mathcal{Q}} f_{\omega} = \Omega^{\mathcal{Q}} - \sum_{\emptyset\neq\omega\in\mathcal{Q}} \mu_{\omega}^{\mathcal{Q}} \frac{\partial\Omega^{\mathcal{Q}}}{\partial\mu_{\omega}^{\mathcal{Q}}} \ . \tag{43}$$

Once more, we have a simple representation for the free energy,

$$-\beta F^{\mathcal{Q}} = \ln Z^{\mathcal{Q}} = -\sum_{\omega\in\mathcal{Q}} \lambda_{\omega}^{\mathcal{Q}} f_{\omega} \ . \tag{44}$$

Again, to determine the $\lambda_{\omega}^{\mathcal{Q}}$ so as to make $p^{\mathcal{Q}}$ satisfy the restricted set (36) of constraints is equivalent to minimizing $\ln Z^{\mathcal{Q}}$ with respect to these parameters or, put differently, over a space of functions $\phi(\kappa)$ which are of the form (41).

Unlike before, the simplicity of (44) need not be purely formal. For instance, if one restricts one's attention to simple approximations which reproduces only a small subset of the set of moments of $q(\kappa)$ — say the translationally invariant expectations $\langle k_a\rangle$ and the translationally invariant nearest neighbour correlations $\langle k_a k_b\rangle$ in the case of bimodal site–disorder, so $\mathcal{Q} = \{\{a\}_{a\in\Lambda}, \{(a,b)\}_{a,b\in\Lambda}\}$, with (a,b) denoting nearest neighbours — then the corresponding Hamiltonian $\mathcal{H}^{\phi}$ acquires only on-site terms and nearest neighbour interactions between the k. So one obtains a fairly simple translationally invariant model. For its study the full machinery of equilibrium statistical mechanics and an established arsenal of approximation methods is, at least in principle, available. We shall demonstrate below that such simple approximations can already yield very precise, if not exact, results.

There are a number of requirements the set $\mathcal{Q}$ should meet to give rise to a sensible approximation for the underlying problem of describing systems with quenched disorder. First, to ensure that the distribution $p^{\mathcal{Q}}$ is normalized, $\mathcal{Q}$ must contain the empty set, since the normalization constraint is expressed precisely by the condition $f_{\emptyset} = \langle k_{\emptyset}\rangle = 1$. Moreover, if the disorder is homogeneous in the sense that the distribution $q(\kappa)$ has a set of moments invariant under the group $\mathcal{G}$ of operations which map the underlying lattice,

hence the set Λ of sites (bonds), onto itself, the set $\mathcal{Q}$ should be such that it respects these symmetries, i.e., it ought to be closed under the operations g of the symmetry group $\mathcal{G}$ of the underlying lattice. Formally, if $\omega \in \mathcal{Q}$ then $g\omega = \{a \in \Lambda;\ g^{-1}a \in \omega\}$ should also be a member of $\mathcal{Q}$. The invariance of the set of moments under $\mathcal{G}$ entails a corresponding invariance of the Lagrangian multipliers, $\lambda^{\mathcal{Q}}_{g\omega} = \lambda^{\mathcal{Q}}_{\omega}$ for all g in $\mathcal{G}$. In other words, the set of constraints can be decomposed into equivalence classes under $\mathcal{G}$.

Fixing $\mathcal{Q}$ so as to concentrate on moments of the disorder distribution which are of finite order or which involve occupation numbers referring to sites (bonds) only up to some maximal distance obviously entails a notion of *locality* for the corresponding disorder potential $\phi^{\mathcal{Q}}(\kappa)$. In what follows, we shall therefore refer to approximations of this type as $\mathcal{Q}$–local.

2.5 Exact Lower Bounds for the Quenched Free Energy

Before turning to a more detailed evaluation of these ideas, let us not fail to mention that the approximative scheme described above provides *exact lower bounds* for the quenched free energy.

This is easily seen by realizing that the constrained entropy maximization scheme described above can be substituted by a constrained minimization scheme for the free energy functional

$$F[p] = \sum_{\sigma,\kappa} p(\sigma,\kappa)\mathcal{H}(\sigma,\kappa) + \beta^{-1} \sum_{\sigma,\kappa} p(\sigma,\kappa) \ln p(\sigma,\kappa) \tag{45}$$

using the set of moments $\langle k_\omega \rangle = f_\omega$, $\omega \in \mathcal{Q}$ as constraints. This yields

$$F[p^{\mathcal{Q}}] = \min_p \Big\{ F[p];\ \langle k_\omega(\kappa) \rangle_p = f_\omega \quad \omega \in \mathcal{Q} \Big\} \ . \tag{46}$$

With suitable Lagrangian multipliers, the $p^{\mathcal{Q}}$ so defined coincides with (40) as obtained from the entropy maximization scheme. If, moreover, one enforces the zero–mean–potential condition (10), then $F[p^{\mathcal{Q}}] = F^{\mathcal{Q}}$, with $F^{\mathcal{Q}}$ given by (44).

The dependece of $F^{\mathcal{Q}}$ on the set $\mathcal{Q} \subseteq \mathcal{P}(\Lambda)$ is *monotone* in the sense that

$$F^{\mathcal{Q}} \leq F^{\mathcal{Q}'} \leq F^{\phi} \quad \text{if } \mathcal{Q} \subseteq \mathcal{Q}' \subseteq \mathcal{P}(\Lambda) \tag{47}$$

so that $F^{\mathcal{Q}}$ approaches the quenced free energy F^{ϕ} monotonically from below, as the set of constraints, as characterized by $\mathcal{Q}$ is increased. A different way to see this is to recall that the $\ln Z^{\mathcal{Q}}$ are obtained by minimizing $\ln Z^{\phi}$ over a space of $\mathcal{Q}$-local functions ϕ — a function space which becomes larger as the set $\mathcal{Q}$ is enlarged.

2.6 Non–Bimodal and Continuous Disorder Distributions and the Variational Content of the Equilibrium Ensemble Approach

The modifications necessary to obtain explicit representations of the disorder potential and approximative schemes for non–bimodal or continuous disorder distributions $q(\kappa)$ can

be inferred from what has been outlined in Secs. 2.3–2.4 above. We will briefly state them in what follows. They also point — more obviously than our previous considerations — to the variational content of the equilibrium ensemble approach to disordered systems.

For the remainder of this section, we drop the restriction that the k_a be bimodal. To begin with, let us assume for simplicity that *all* moments of the (non–bimodal or continuous) disorder distribution $q(\kappa)$ exist. They are given as expectations under $q(\kappa)$ of all possible products of powers of the k_a, *i.e.*, by

$$f_\omega^{\boldsymbol{n}} = \left\langle \prod_{a\in\omega} k_a^{n_a}(\kappa) \right\rangle_q \qquad , \ \omega \in \Lambda, \ n_a \in I\!N \ , \tag{48}$$

with $\boldsymbol{n} = (n_a)_{a\in\omega}$. The partition function of the equivalent equilibrium ensemble describing the disordered system is then given by

$$Z^\phi = \sum_{\sigma,\kappa} \exp[-\beta\mathcal{H}(\sigma|\kappa) - \beta\phi(\kappa)] \ , \tag{49}$$

with ϕ of the form

$$\beta\phi(\kappa) = \sum_{\omega\subseteq\Lambda,\boldsymbol{n}} \lambda_\omega^{\boldsymbol{n}} (k_\omega^{\boldsymbol{n}}(k) - f_\omega^{\boldsymbol{n}}) \ . \tag{50}$$

Here we have introduced

$$k_\omega^{\boldsymbol{n}}(\kappa) = \prod_{a\in\omega} k_a^{n_a}(\kappa) \ . \tag{51}$$

In (49), (50) we have chosen to satisfy the zero–mean–potential condition (10) at the outset. The coupling constants $\lambda_\omega^{\boldsymbol{n}}$ have to be determined such that the Gibbs distribution p^ϕ corresponding to (49) reproduces the moments of the underlying disorder distribution q, *i.e.*, $\langle k_\omega^{\boldsymbol{n}}\rangle = f_\omega^{\boldsymbol{n}}$ is supposed to hold for all ω and $\boldsymbol{n}$. This amounts to minimize $\ln Z^\phi$ as a function of the $\lambda_\omega^{\boldsymbol{n}}$, in complete analogy with the bimodal case. As above, the $\lambda_\omega^{\boldsymbol{n}}$ can be interpreted as Lagrangian multipliers of a constrained entropy maximiation scheme or, alternatively, of a constrained free energy minimization scheme.

As before, approximations are obtained by enforcing only a subset of the full set of constraints, that is, by requiring the Gibbs distribution p^ϕ to reproduce only a subset of the full set of moments (48) of the disorder distribution $q(\kappa)$. This can be done in several ways, for instance by requiring a match with the $f_\omega^{\boldsymbol{n}}$ only for ω in some subset $\mathcal{Q}$ of the powerset $\mathcal{P}(\Lambda)$ of the set of sites (or bonds) of the lattice, by matching moments only up to some maximal value for the n_a, or by combining these two truncation schemes in various ways.

If one defines the approximations through a moment matching scheme restricted *only* with respect to the choice of the ω in (48) and (50), demanding that $\omega \in \mathcal{Q} \subseteq \mathcal{P}(\Lambda)$ as in Sec. 2.4, the minimization of $\ln Z^\phi$ with respect to the correspondingly restricted set of parameters $\lambda_\omega^{\boldsymbol{n}}$, $\omega \in \mathcal{Q}$, amounts to a minimization over a true infinite dimensional function space, *i.e.*, as a variational problem. It amounts to minimizing $\ln Z^\phi$, interpreted as a functional of ϕ over a space of functions ϕ which are $\mathcal{Q}$–*local* in the sense defined above. That is, they are of the form

$$\phi(\kappa) = \sum_{\emptyset\neq\omega\in\mathcal{Q}} \Big(\psi_\omega(\kappa) - \langle\psi_\omega(\kappa)\rangle_q\Big) \ , \tag{52}$$

each ψ_ω being a function of the k_a, $a \in \omega$, which is analytic in every component, since power series expansions were assumed to exist; cf. Eq. (50). Restricting also the range of n_a values would further restrict the set of functions to multinomials of some maximal degree.

Conversely, dropping the analyticity constraint on the ψ_ω will enlarge the function space sufficiently to treat cases where *not* all moments of $q(\kappa)$ exist.

Having said this much, it should have become clear that the equivalent equilibrium ensemble approach could have been formulated as a variational problem right away. To wit, consider Z^ϕ, interpreted as a functional of ϕ,

$$Z^\phi = Z[\phi] = \sum_\kappa Z(\kappa) \exp[-\beta\phi(\kappa)], \tag{53}$$

and let us assume at the outset that the ϕ under consideration satisfy the zero–mean–potential condition (10); alternatively, one might impose it a–posteriori. Using the disorder distribution $q(\kappa)$ this may be rewritten as an average:

$$Z^\phi = Z[\phi] = \langle Z(\kappa) \exp[-\beta\phi(\kappa) - \ln q(\kappa)] \rangle_q \ . \tag{54}$$

By Jensen's inequality,

$$\ln Z^\phi = \ln Z[\phi] \geq \langle \ln Z(\kappa) \rangle_q - \langle \ln q(\kappa)] \rangle_q \ , \tag{55}$$

where we have invested $\langle \phi(\kappa) \rangle_q = 0$. The task then is to minimize the left hand side of (55) over a suitable space of functions ϕ satisfying $\langle \phi(\kappa) \rangle_q = 0$. This variational point of view was utilized by George *et al.* [10] in their study devoted to the computation of phase–boundaries of bond–disordered 2–D Ising models — without connecting it to the equilibrium ensemble idea and to the heuristics associated with it, and without, so it seems, the awareness that it allows to proceed to exact solutions.

Indeed, the inequality in (55) can be satisfied as an equality, *i.e.*, the lowest bound attained and thereby the exact quenched free energy computed, if $\phi(\kappa)$ is chosen such that

$$Z(\kappa) \exp[-\beta\phi(\kappa) - \ln q(\kappa)] = \text{const} \tag{56}$$

in the sense that this quantity does not depend on κ. The value of this constant must, of course, be Z^ϕ, so (56) is nothing but the Morita equation (6) in disguise. That is, it is the formal solution of the variational problem

$$\frac{\delta \ln Z[\phi]}{\delta \phi} = 0 \ . \tag{57}$$

Approximations are obtained by restricting the space of functions ϕ over which a minimum of $\ln Z[\phi]$ is sought, in other words, the domain of defenition of the functional $\ln Z[\phi]$, to functions which are $\mathcal{Q}$–local in the sense explained before. Approximations can systematically be improved by increasing the size of the set $\mathcal{Q}$

3 Recursive evaluation of coupling constants

For systems with quenched, uncorrelated bimodal site or bond disorder, one can write down more or less explicit expressions for the coupling constants λ_ω of the full disorder potential ϕ. It turns out that these expressions generate conventional low–concentration expansions for the quenched free energy (1) as well as perturbation expansions about pure reference systems. In the present section, we shall establish this connection. In Sec. 3.2, we specialize to models with bond– or site–dilution for which additional exact information about the exact disorder potential $\phi(\kappa)$ is available. Among other things, we use it to reproduce the known exact solutions of one–dimensional models with quenched site or bond dilution and to exhibit simplifying features of these solutions in the absence of symmetry breaking fields.

3.1 General results

We consider systems with quenched, uncorrelated bimodal site or bond disorder, defined on a lattice $\mathcal{L}$ containing N sites. As before, let Λ denote the set of sites (bonds) of the lattice. The distribution $q(\kappa)$ describing the disorder configurations

$$\kappa = \{k_a;\ a \in \Lambda\} \equiv \{a \in \Lambda;\ k_a = 1\} \tag{58}$$

is characterized by a single parameter ρ,

$$q(\kappa) = \prod_{a \in \Lambda} \rho^{k_a} (1-\rho)^{1-k_a} = \rho^{|\kappa|} (1-\rho)^{|\Lambda|-|\kappa|} \ , \tag{59}$$

so that

$$f_\omega = \langle k_\omega \rangle_q = \rho^{|\omega|}. \tag{60}$$

We use the Morita equation (6),

$$\beta\phi(\kappa) = -\ln[q(\kappa)/Z(\kappa)] - \ln Z^\phi \tag{61}$$

and the representation

$$\beta\phi(\kappa) = -\sum_{\emptyset \neq \omega \subseteq \Lambda} \lambda_\omega (k_\omega(\kappa) - f_w) \tag{62}$$

for the exact potential $\phi(\kappa)$, to obtain the coupling constants λ_ω. This is achieved by inserting (62) and (60) into the Morita equation, and by considering this equation first for $\kappa = \emptyset$, which gives

$$\beta\phi(\emptyset) = \sum_{\emptyset \neq \omega \subseteq \Lambda} \lambda_\omega \rho^{|\omega|} = -|\Lambda| \ln(1-\rho) + \ln Z(\emptyset) - \ln Z^\phi \ , \tag{63}$$

and then for $\kappa \neq \emptyset$, which yields

$$\begin{aligned} \beta\phi(\kappa) &= \beta\phi(\emptyset) - \sum_{\emptyset \neq \omega \subseteq \kappa} \lambda_\omega \\ &= -|\Lambda| \ln(1-\rho) - |\kappa| \ln\left[\frac{\rho}{1-\rho}\right] + \ln Z(\kappa) - \ln Z^\phi \ . \end{aligned} \tag{64}$$

Subtracting (64) from (63), we get

$$\sum_{\emptyset\neq\omega\subseteq\kappa}\lambda_\omega = -|\kappa|\ln\left[\frac{1-\rho}{\rho}\right] - \ln Z(\kappa) + \ln Z(\emptyset)\ , \quad \forall\ \kappa\neq\emptyset\ . \tag{65}$$

To determine the λ_ω individually, we introduce the quantities x_ω, $\omega\subseteq\Lambda$, through

$$Z(\kappa) = \prod_{\omega\subseteq\kappa} x_\omega \tag{66}$$

or, equivalently

$$\ln Z(\kappa) = \sum_{\omega\subseteq\kappa}\ln x_\omega\ , \tag{67}$$

where κ ranges through all subsets of Λ (including the empty set) and the product in (66) is over all subsets of κ, including again the empty set. Eq. (66) may be interpreted as a *recursive definition* of the x_ω; alternatively, one may invert this relation directly to yield

$$\ln x_\omega = \sum_{\kappa\subseteq\omega}(-)^{|\omega|-|\kappa|}\ln Z(\kappa)\ . \tag{68}$$

Inserting this into (65), and recalling that (65) is supposed to hold for *all* $\kappa\neq\emptyset$, we can immediately conclude

$$\lambda_\omega = -\ln\left[x_\omega\Big(\frac{1-\rho}{\rho}\Big)^{\delta_{|\omega|,1}}\right]\ , \quad \omega\neq\emptyset\ . \tag{69}$$

This is the more or less explicit expression for the coupling constants λ_ω of the exact disorder potential ϕ announced above. Using this result, and returning, once more, to the $\kappa=\emptyset$ version (63) of the Morita equation, we get an (again more or less explicit) expression for the free energy of the equivalent equilibrium ensemble,

$$\ln Z^\phi = -|\Lambda|[\rho\ln\rho + (1-\rho)\ln(1-\rho)] + \sum_{\omega\subseteq\Lambda}\rho^{|\omega|}\ln x_\omega\ . \tag{70}$$

The first contribution in (70) is readily identified as the expected contribution of the entropy of mixing. Using (68), the second contribution can be cast into the form

$$\sum_{\omega\subseteq\Lambda}\rho^{|\omega|}\ln x_\omega = \sum_{\kappa\subseteq\Lambda}\rho^{|\kappa|}(1-\rho)^{|\Lambda|-|\kappa|}\ln Z(\kappa)\ . \tag{71}$$

Up to the factor $-\beta^{-1}$ this is just the Brout avarage (1) of the free energy for the case of quenched, uncorrelated bimodal site or bond disorder as it should, since no approximations were involved in the above considerations.

Clearly, we cannot expect to be able to evaluate (70) completely, if we are unable to do so in the more standard formulation (11). Nevertheless, we have gained something useful.

First, Eq. (70) together with (68) amounts to a formal model–independent prescription for reorganizing the Brout average in such a way that it is turned into an expansion ordered by increasing powers of ρ. That is, for systems with bimodal bond– or site–disorder, there is apparently an intimate relation between the equilibrium ensemble approach to

disordered systems and conventional low concentration expansions for such systems. It should be noted that we were as yet not forced to specify the physical meaning of (low) concentration in the above considerations. Clearly, this will depend on which meaning we decide to associate with the $k_a = 1$ states of the disordered system. Think for example of a randomly spin–diluted magnet. If we choose $k_a = 1$ to designate that site a is occupied by a spin, then ρ has the meaning of a (spin) density, and (70) gives indeed a conventional low concentration expansion. We might, of course, also have chosen $k_a = 1$ to designate an empty site (occupation by a vacancy), thereby generating an expansion about the pure, homogeneous reference system. Clearly these different choices are giving entirely different meanings to the expressions appearing in (68), (70) and (71). The quantity $x_\emptyset = \ln Z(\emptyset)$, for instance, gives the free energy of the empty lattice, if $k_a = 1$ denotes occupancy by a spin, whereas it gives the free energy of the fully occupied homogeneous system, if $k_a = 1$ denotes that site a is empty.

Second, we can use the formal results obtained above to compute at least the simplest coupling constants of the exact disorder potential explicitly. This turns out to provide useful information for the investigation of the approximative systems introduced in the previous subsection.

Third, for models with bond– or site–dilution, we will be able to show in Sec. 3.2 below, that a large nontrivial class of coupling constants of the exact disorder potential ϕ will vanish in the absence of symmetry-breaking fields. This piece of information, too, can be useful as a guide for finding efficient sequences of approximations within the scheme presented in Sec. 2.4.

3.2 Models with Bond– and Site–Dilution

Models with bond– and site–dilution exhibit a simplifying feature which allows to carry the formal developement of the equilibrium ensemble approach one step further, namely the notion of independent non–interacting clusters in terms of which every disorder configuration can be characterized.

If we adopt the convention that $k_a = 1$ denotes an occupied site (bond), so that the equilibrium ensemble approach generates a conventional low concentration expansion as explained in the previous subsection, we can establish the following results:

(i) $x_\omega = 1$, hence $\lambda_\omega = 0$, if ω denotes a *disconnected* set of occupied sites (bonds).

(ii) In the absence of symmetry breaking fields, $x_{\omega \cup \{a\}} = 1$, hence $\lambda_{\omega \cup \{a\}} = 0$, if ω denotes a connected cluster containing at least two occupied sites (one occupied bond) to which a single site (bond) a is added to form a *dangling* connection with ω.

(iii) In the absence of symmetry breaking fields, $x_{\omega_1 \cdot \omega_2} = 1$, hence $\lambda_{\omega_1 \cdot \omega_2} = 0$, if $\omega_1 \cdot \omega_2$ denotes a connected cluster of sites (bonds) which consists of two separate sub–clusters ω_1 and ω_2 that are conneted only via a single common site.

Note that (ii) can in fact be read as a special case of (iii). All three results hold for site or bond diluted models with nearest neighbour interactions on arbitrary graphs. They

follow directly from the definition (66) of the x_ω. We establish them separately for systems with site–dilution and with bond–dilution.

3.2.1 Models with site–dilution

Identifying the configurations κ of the disordered system with the sets of occupied sites, we have

$$Z(\emptyset) = x_\emptyset = 1 \ , \tag{72}$$

and

$$Z(\kappa) = \prod_{\emptyset \neq \omega \subseteq \kappa} x_\omega \tag{73}$$

for $\kappa \neq \emptyset$. The proof of (i) is by induction. First, using $Z(\{a\}) = x_{\{a\}} = Z_1$ for configurations in which only a single site a is occupied, and $Z(\{a\} \cup \{b\}) = Z(\{a\})Z(\{b\}) = Z_1^2$, if a and b are not nearest neighbours, one immedieately obtains $x_{\{a,b\}} = 1$ for the simplest disconnected set $\{a, b\}$ containing only two sites. Supposing now that (i) has been proven for *all* disconnected sets ω containing up to n sites, and assuming that κ denotes a disconnected site containig $n + 1$ sites, one has

$$Z(\kappa) = \prod_{\kappa_\alpha \subseteq \kappa} Z(\kappa_\alpha) \ , \tag{74}$$

where the product is over all independent clusters (maximally connected subsets) of κ. By supposition

$$Z(\kappa) = \prod_{\kappa_\alpha \subseteq \kappa} Z(\kappa_\alpha) = \prod_{\kappa_\alpha \subseteq \kappa} \Big(\prod_{\omega_\alpha \subseteq \kappa_\alpha} \omega_\alpha \Big) \, x_\kappa \tag{75}$$

entailing $x_\kappa = 1$ also for the disconnected set κ containing $n + 1$ sites, which proves (i) for the case of site–dilution.

Next, to prove (ii) we consider configurations of the form $\kappa = \omega \cup \{a\}$, where the site a forms a *dangling connection* with ω. Denote by $E(\sigma_a, \sigma_b)$ the interaction energy between the degree of freedom sitting on the dangling site a and σ_b, the degree of freedom in ω to which it is connected, in the absence of symmetry breaking fields. This interaction energy is assumed to be invariant under an internal symmetry group of the model in the sense that

$$\hat{Z} = \sum_{\sigma_a} \exp[-\beta E(\sigma_a, \sigma_b)] \tag{76}$$

is *independent* of σ_b so that the partition function $Z(\kappa) = Z(\omega \cup \{a\})$ in the absence of symmetry breaking fields is given by

$$Z(\kappa) = Z(\omega \cup \{a\}) = \hat{Z} \ Z(\omega) \ . \tag{77}$$

The proof of (ii) is likewise by induction. First, we have $Z(\{a\}) = Z_1 = x_{\{a\}}$ and, by the factorizing property (77), $Z(\{a, b\}) = Z_2 = \hat{Z} \ Z_1 = x_{\{a\}}^2 \ x_{\{a,b\}}$ for a configuration containing only two neighbouring sites a and b. This gives $x_{\{a,b\}} = \hat{Z}/Z_1$. Adding another dangling connection in $\kappa = \{a, b, c\}$ gives $Z(\{a, b, c\}) = Z_3 = \hat{Z}^2 \ Z_1 = x_{\{a\}}^3 \ x_{\{a,b\}}^2 \ x_{\{a,b,c\}}$, so $x_{\{a,b,c\}} = 1$, which verifies (ii) for the smallest conceivable set of the form $\omega \cup \{a\}$ with

ω containing two sites. Suppose now that (ii) has been established for all sets of the form $\omega \cup \{a\}$ with a dangling connection from ω to a single site a and with ω containing up to n sites, and let κ be of the form $\kappa = \tilde{\omega} \cup \{a\}$ with $\tilde{\omega}$ containing $n+1$ sites. Then

$$\begin{aligned} Z(\kappa) &= Z(\tilde{\omega} \cup \{a\}) = \hat{Z}\ Z(\tilde{\omega}) \\ &= \Big(\prod_{\emptyset \neq \omega \subseteq \tilde{\omega}} x_\omega \Big) \Big(\prod_{\emptyset \neq \omega' \subset \tilde{\omega}} x_{\omega' \cup \{a\}} \Big)\ x_{\{a\}}\ x_{\tilde{\omega} \cup \{a\}}\ , \end{aligned} \tag{78}$$

so

$$\hat{Z} = \Big(\prod_{\emptyset \neq \omega' \subset \tilde{\omega}} x_{\omega' \cup \{a\}} \Big)\ x_{\{a\}}\ x_{\tilde{\omega} \cup \{a\}}\ . \tag{79}$$

By supposition all $x_{\omega' \cup \{a\}}$ in the above product except $x_{\{a,b\}}$ are unity, where b denotes the unique site in $\tilde{\omega}$ connected to a via the dangling connection. Since $x_{\{a,b\}}\ x_{\{a\}} = \hat{Z}$, we can conclude that $x_{\tilde{\omega} \cup \{a\}} = 1$ as well, which completes the proof of (ii) for the site–diluted system.

To verify (iii), note that the result $x_{\{a,b,c\}} = 1$ for three neighbouring sites a, b, c obtained above establishes (iii) for the smallest conceivable set of the form $\omega_1 \cdot \omega_2$, with $\omega_1 = \{a, b\}$ and $\omega_2 = \{b, c\}$. The result follows by induction after noting that in the absence of symmetry breaking fields $Z(\omega_1 \cdot \omega_2) = Z_1^{-1} Z(\omega_1) Z(\omega_2)$, and by considering the consequences of this identity in the x_ω–representation.

3.2.2 Models with bond–dilution

In the bond–diluted case, we identify κ with the set of occupied bonds. Thus, if $\kappa = \emptyset$, the system consists of a collection of N non–interacting degrees of freedom, and hence

$$Z(\emptyset) = Z_1^N\ , \tag{80}$$

where, as before, Z_1 denotes the parition function of an isolated degree of freedom. If $\kappa \neq \emptyset$, there will be a set of *interacting* degrees of freedom — those sitting in clusters formed by bonds occupied in κ — but in general also a collection of non–interacting degrees of freedom. Denoting by Z_κ the partition function of the degrees of freedom *interacting* through the set of bonds occupied in κ, we can write

$$Z(\kappa) = Z_1^N\ \frac{Z_\kappa}{Z_1^{n(\kappa)}} \equiv Z_1^N\ \tilde{Z}(\kappa)\ , \tag{81}$$

where $n(\kappa)$ is the number of vertices linked by bonds occupied in κ. Returning to the x_ω representation (66), we identify

$$x_\emptyset = Z_1^N \tag{82}$$

and

$$\tilde{Z}(\kappa) = \frac{Z_\kappa}{Z_1^{n(\kappa)}} = \prod_{\emptyset \neq \omega \subseteq \kappa} x_\omega\ . \tag{83}$$

The $\tilde{Z}(\kappa)$ have properties analogous to the $Z(\kappa)$ in the site–diluted problem. In particular, if $\kappa = \kappa_1 \cup \kappa_2$ and κ_1 and κ_2 are mutually disconnected sets of occupied bonds, then $\tilde{Z}(\kappa) =$

$\tilde{Z}(\kappa_1)\tilde{Z}(\kappa_2)$. This factorizing property again entails $x_\omega = 1$, if ω denotes a disconnected set of bonds. The proof is by induction in complete analogy to the site diluted case, and it will not be repeated here.

Next, to establish (ii) for the bond diluted case, we note that

$$\tilde{Z}(\omega \cup \{a\}) = \frac{Z_{\omega\cup\{a\}}}{Z_1^{n(\omega)+1}} = \frac{\hat{Z}}{Z_1}\frac{Z_\omega}{Z_1^{n(\omega)}} = \frac{\hat{Z}}{Z_1}\tilde{Z}(\omega) \tag{84}$$

in the absence of symmetry breaking fields, if a denotes a dangling connection added to the set ω; here $\hat{Z}$ has the same meaning as in the site diluted case. Again, by inductive reasoning in complete analogy with the site diluted problem, one verifies (ii), i.e., $x_{\omega\cup\{a\}} = 1$ if ω contains at least one occupied bond.

Finally, to prove (iii), we note that

$$\tilde{Z}(\omega_1 \cdot \omega_2) = \frac{Z_{\omega_1\cdot\omega_2}}{Z_1^{n(\omega_1)+n(\omega_2)-1}} = \frac{Z_{\omega_1}}{Z_1^{n(\omega_1)}}\frac{Z_{\omega_2}}{Z_1^{n(\omega_2)}} = \tilde{Z}(\omega_1)\tilde{Z}(\omega_2) \ , \tag{85}$$

where the second equality requires the absence of symmetry breaking fields. This factorizing property of the $\tilde{Z}(\omega_1 \cdot \omega_2)$ entails (iii) on the level of the x_ω–representation.

3.2.3 One dimensional models with bond– or site–dilution

One dimensional systems with bond or site dilution are particularly simple because in 1–d one has a complete overview over the family of connected clusters which consists just of isolated (finite) chains. This allows to give an explicit representaion of the x_ω defined through (66) in terms of chain free energies, which we briefly record here.

For the site diluted problem, denoting by Z_n the partition function of an isolated open chain of n occupied sites, and by x_n the corresponding x variable, we have

$$Z_n = \prod_{k=1}^{n} x_k^{n+1-k} \ , \tag{86}$$

which gives $x_1 = Z_1$, and (with $Z_0 = 1$)

$$x_n = Z_n Z_{n-2}/Z_{n-1}^2 \ , \qquad n \geq 2 \ . \tag{87}$$

Inserting this into the expression (70) for the free energy of the equivalent equilibrium ensemble and normalizing with respect to sample size $N = |\Lambda|$, we get

$$\begin{aligned} -\beta f^\phi &= \lim_{N\to\infty} N^{-1} \ln Z^\phi \\ &= -\rho \ln \rho - (1-\rho)\ln(1-\rho) + (1-\rho)^2 \sum_{n=1}^{\infty} \rho^n \ln Z_n \ . \end{aligned} \tag{88}$$

Up to the contribution coming from the entropy of mixing, this reproduces the exact solution as obtained, e.g., by Wortis [25]. In the absence of symmetry breaking fields we have $\ln x_n = 0$ for $n \geq 3$, so in this case

$$-\beta f^\phi = -\rho \ln \rho - (1-\rho)\ln(1-\rho) + \rho \ln Z_1 + \rho^2 \ln(Z_2/Z_1^2) \ . \tag{89}$$

In the bond diluted problem, isolateds chain containing n successive bonds constitute chains of $n+1$ interacting degrees of freedom. If we formulate (83) for such chains, it reads

$$\frac{Z_{n+1}}{Z_1^{n+1}} = \prod_{k=1}^{n} x_k^{n+1-k} \ , \tag{90}$$

where the x_k now refer to chains containing k *bonds*. This gives $x_1 = Z_2/Z_1^2$, and

$$x_n = Z_{n+1} Z_{n-1}/Z_n^2 \ , \qquad n \geq 1. \tag{91}$$

Comparing with the corresponding expression (87) for the site–diluted case, we note that $x_n^{\rm bond} = x_{n+1}^{\rm site}$ for $n \geq 1$. For the free energy per site in the bond–diluted system we thus get (recalling $x_\emptyset = Z_1^N$)

$$-\beta f^\phi = -\rho \ln \rho - (1-\rho)\ln(1-\rho) + (1-\rho)^2 \sum_{n=1}^{\infty} \rho^{n-1} \ln Z_n \ , \tag{92}$$

thereby reproducing again the exact solution[25]. In the absence of symmmetry breaking fields, $\ln x_n = 0$ for $\nu \geq 2$, and the expression simplifies to

$$-\beta f^\phi = -\rho \ln \rho - (1-\rho)\ln(1-\rho) + \ln Z_1 + \rho \ln(Z_2/Z_1^2) \ . \tag{93}$$

Eqs. (88) and (92) can be evaluated for all models for which the finite chain thermodynamics is known, e.g., from transfer–matrix techniques.

Note that the result (ii) concerning the vanishing of coupling constants of the disorder potential of the form $\lambda_{\omega \cup \{a\}}$ in the absence of symmetry breaking fields implies that in this limit very simple approximations in the moment–matching approximation scheme described in Sec. 2.2 already provide *exact* solutions for bond– or site–diluted chains. For the bond–diluted case, it is the simplest conceivable annealed approximation enforcing only the average occupancy $\langle k_a \rangle = \rho$ of the bonds. In the case of site–dilution, one has to fix the average site–occupancy at ρ and the expectations $\langle k_a k_b \rangle$ for neighbouring sites at ρ^2 in order to reproduce the thermodynamics of the quenched system exactly.

On the contrary, if there *is* a nonvanishing symmetry breaking field, then Eqs. (87) and (91) imply that *no finite approximation* in the moment–matching scheme described in Sec. 2.2 is exact. Nevertheless, the simplest approximations enforcing only $\langle k_a \rangle = \rho$ in the bond–diluted case, and both, the site occupancy $\langle k_a \rangle = \rho$ and the nearest neighbour expectation $\langle k_a k_{a+1} \rangle = \rho^2$ in the site–diluted case already give rather precise results, as will be demonstrated for the Ising model in II.

4 Thermally Correlated Frozen-In Disorder

Having treated uncorrelatded bimodal bond– and site–disorder in some detail, it is perhaps appropriate to recall that the equlibrium ensemble approach to disordered systems is not restricted to this case. Except in the previous section we have, in fact, never made use of the specific simplifications pertaining to uncorrelated disorder. The moment matching schemes explaind in Secs. 2.4–2.6. can naturally also be put to work in the case of *correlated*

disorder. The only nontrivial piece of information needed is contained in the system of moments (20) or (48) for the bimodal and non-bimodal cases, respectively. In real physical systems, which *do* as a rule exhibit some degree of correlations between the configurational degrees of freedom, a subset of the full set of moments, obtained *e.g.* through scattering experiments, is often the only piece of information that is actually available about the disordered system in question. So, in situations where relatively simple approximations in a moment matching scheme can be expected to produce reliable results, the equilibrium ensemble approach appears to be an ideally suited tool to use.

In the present section we will treat *correlated* bimodal bond– and site–disorder in some detail. We will restrict our attention to the case where the correlations are produced as a result of some previous annealing proccess (in the narrow metallurgical sense). That is, we suppose that the quenched disorder distribution is an equilibrium distribution produced at values of the external parameters (temperature, fields, chemical potential, etc.) characteristic of the preparation process, but in general different from the values at which experiments on the system are actually being perfomed.

Let us assume that the system is prepared at (inverse) temperature $\bar{\beta}$ and that it is described by the total Hamiltonian

$$\bar{\mathcal{H}}_{\rm tot}(\sigma,\kappa) = \bar{\mathcal{H}}(\sigma|\kappa) + V(\kappa) \tag{94}$$

where $\bar{\mathcal{H}}(\sigma|\kappa)$ is the Hamiltonian of the disordered system describing the energy of the σ–degrees of freedom at fixed disorder configuration κ, albeit at parameter settings characteristic of the preparation process, which we indicate by the overbar. The potential $V(\kappa)$ accounts for the fact that there may be an additional interaction energy between the configurational degrees of freedom which produces correlations between the k_a over and above that mediated by σ. Think, for example, of a dilute magnetic alloy. The distribution of particles will usully be governed, both, by chemical interactions — accounted for by $V(\kappa)$ — and by κ–dependent interactions between magnetic degrees of freedom described by $\bar{\mathcal{H}}(\sigma|\kappa)$. In typical cases, the former may, in fact, be expected to dominate.

We assume that during the preparation process the temperature is high enough to allow the system to come to complete equilibrium. The distribution of the configurational degrees of freedom is then given by

$$\bar{q}(\kappa) = \frac{\bar{Z}(\kappa)}{\bar{Z}} \exp[-\bar{\beta}V(\kappa)] \ , \tag{95}$$

where $\bar{Z}(\kappa) = \sum_\sigma \exp[-\bar{\beta}\bar{\mathcal{H}}(\sigma|\kappa)]$. If the system is then cooled down to lower temperatures, the impurity distribution (95) may be regarded as fixed, and the disordered system characterized by this quenched distribution will exhibit frozen correlations between impurities. In what follows, we will show that the formal developments presented in Sec. 3 for the uncorrelated case can be carried almost as far in the case of thermally correlated quenched disorder.

To this end we return to the Morita equation (6) and the representation

$$\beta\phi(\kappa) = -\sum_{\emptyset\neq\omega\subseteq\Lambda} \lambda_\omega (k_\omega(\kappa) - \bar{f}_w) \tag{96}$$

of the disorder potential $\phi(\kappa)$, the overbar indicating that the moments are evaluated with (95).

The coupling constants of the disorder potential for this problem of correlated disorder can now be determined along the same lines as in Sec. 3.1. For the bimodal disorder type considered here, we can always write

$$V(\kappa) = \sum_{\omega \subseteq \Lambda} v_\omega k_\omega(\kappa) \tag{97}$$

Using the x representation (66) for both $Z(\kappa)$ and for the partition function $\bar{Z}(\kappa)$ with the parameters settings prevalent during the preparation process, we get

$$\lambda_\omega = -\bar{\beta} v_\omega - \ln(x_\omega / \bar{x}_\omega) \quad , \quad \omega \neq \emptyset \ . \tag{98}$$

Returning to the $\kappa = \emptyset$–version of the Morita equation, and recalling that $\bar{f}_\emptyset = 1$ irrespectively of the correlations, and that $Z(\emptyset) = x_\emptyset$ and similarly $\bar{Z}(\emptyset) = \bar{x}_\emptyset$, the free energy F^ϕ is obtained in the form

$$\begin{aligned} -\beta F^\phi &= \ln Z^\phi = \ln \bar{Z} + \sum_{\omega \subseteq \Lambda} (\bar{\beta} v_\omega + \ln(x_\omega / \bar{x}_\omega)) \bar{f}_\omega \\ &= -\langle \ln \bar{q}(\kappa) \rangle_{\bar{q}} + \sum_{\omega \subseteq \Lambda} \ln x_\omega \bar{f}_w \ . \end{aligned} \tag{99}$$

The reader is invited to compare this with (70). The main additional obstacle on the way to evaluating the moment expansion (99) to high orders — assuming such an evaluation were possible for the concentration expansion(70) in the uncorrelated case — lies in the $\bar{f}_\omega$, which cannot be expected to be of such a simple form as in the case of uncorrelated disorder. Nevertheless, analytic approximations are conceivable in the form of high–temperature expansions of the $\bar{f}_\omega$, if $\bar{\beta}$ is sufficiently small. In any case, as will be shown in II, relatively simple moment matching schemes, that is, simple approximations in the restricted annealing approach, which do not require knowledge of high moments, may still be feasible and useful.

It should be noted that the disorder potential $\phi(\kappa)$ reduces to $V(\kappa)$, if parameter values are the same as those during system preparation, so that $x_\omega = \bar{x}_\omega$. The reader may convince herself that this just what is needed produce the correct limiting form of Z^ϕ in the case where $\bar{q}(\kappa)$ is the equilibrium distribution of the configurational degrees of freedom κ.

Specializing to systems with bond– or site–dilution, we observe that the results concerning the vanishing of certain coupling constants of the disorder potential ϕ stated and proved in Sec. 3.2 have simple analogues in the case of thermally correlated disorder. To see this, note that the results (i)–(iii), if formulated on the level of the x_ω, do not depend on disorder statistics or parameter settings; so they hold for the $\bar{x}_\omega$ alike. For thermally correlated quenched disorder, statements to the end that $x_\omega = \bar{x}_\omega = 1$ then translate into $\lambda_\omega = -\bar{\beta} v_\omega$. This implies a vanishing of the coupling constants as in the uncorrelated case, if the the potential $V(\kappa)$ involves no interactions beyond those coupling configurational degrees of freedom on neighbouring sites (bonds).

Taking site–diluted chains in the absence of symmetry breaking fields as an example, we obtain the following surprisingly simple expression for the free energy per site as computed in the equilibrium ensemble approach,

$$-\beta f^{\phi} = k_{\mathrm{B}}^{-1}\bar{s}_0 + \bar{f}_1 \ln Z_1 + \bar{f}_2 \ln(Z_2/Z_1^2) \ , \tag{100}$$

where $\bar{s}_0$ is the entropy of mixing per site, while $\bar{f}_1 = \langle k_a \rangle_{\bar{q}} = \rho$ and $\bar{f}_2 = \langle k_a k_{a+1} \rangle_{\bar{q}}$. That is all effects of quenched correlations on the free energy of the system make themselves felt *only* through the modified nearest neighbour correlation. This ceases to be the case if a symmetry breaking field is applied. Note that symmetry breaking fields during the preparation process manifest themselves in this context — beyond their effect in modifying $\bar{f}_1$ and $\bar{f}_2$ — only in modifying the entropy of mixing.

Similarly, in the bond–diluted system with thermally correlated quenched bond occupancy one obtains

$$-\beta f^{\phi} = k_{\mathrm{B}}^{-1}\bar{s}_0 + \ln Z_1 + \bar{f}_1 \ln(Z_2/Z_1^2) \ . \tag{101}$$

So the result depends only on the average occupancy $\bar{f}_1 = \rho$ of the bonds and is *independent* of correlations between them.

The simplicity of the zero–field solutions (100) and (101) for the 1–D systems with quenched thermal correlations is not easily detected in the exact solution [26], which has been obtained by the direct averaging approach.

5 Concluding Remarks

We have presented an outline of the formal and systematic aspects of Morita's equilibrium ensemble approach to systems with quenched disorder [6]. Hitherto unnoticed relations to other, more conventional sets of ideas, such as low concentration expansions, perturbation expansions about pure reference systems, variational bounding of free energies, and generalizations of the idea of grand ensembles have been pointed out and elaborated.

The *canonical* approximation scheme within Morita's approach — a moment matching procedure that goes under the name of restricted or constrained annealing — is of a *non–perturbative* nature, which should also be clear in view of its relation to variational methods. Conversely, the expansion of the *exact* disorder potential was demonstrated to generate conventional perturpation expansions. A third, in some sense intermediate approach would be to attempt solving or analysing models with a truncated expansion of the full disorder potential exactly.

For models with bond– or site–dilution, it was demonstrated that a large non–trivial class of coupling constants of the exact disorder potential $\phi(\kappa)$ vanishes in the absence of symmetry–breaking fields. This fact may help to explain why relatively simple approximations within the moment matching schemes or the variational formulation presented in Sec. 2 have been so successful in describing aspects of critical behaviour of *e.g.* disordered Ising models — undisputably so at least regarding the computation of phase transition lines ([8], [9], [10], [17]), still under debate though (see, *e.g.*, [27]), regarding the much more controversial and difficult question of critical exponents [17], [22].

In the case of continuous disorder distributions, straightforward moment matching schemes as explained in Sec. 2 might not always prove to be the most efficient way of formulating approximative solutions. Instead of fixing moments up to a certain order directly, one might, for instance think of reproducing expectations only of certain *combinations* of moments of the quenched disorder distribution in the equilibrium ensemble. The choice of particular combinations might be guided by attempts to exploit powerful analytic structures, such as provided by orthogonal function systems, or by physical insight. In bond–disordered Ising models, for instance, the representation of the exact solution in terms of weighted sums over configurations of van der Waerden polygons suggests that the decisive quantities to be reproduced in an equilibrium ensemble approach would be gauge–invariant loop-correlations of the natural high–temperature variables $t_{ij} = \tanh(\beta J_{ij})$, expressed here in terms of the conventional notation for the exchange couplings. That is, the disorder potential $\phi(\kappa) \equiv \phi(\{t_{ij}\})$ would be designed to fix correlations of the t_{ij} around closed loops $\mathcal{C}$, *i.e.*, correlations of the form $\left\langle \prod_{(i,j)\subset\mathcal{C}} t_{ij} \right\rangle$ at their corresponding quenched values, each such correlation involving moments of the corresponding quenched $\{J_{ij}\}$–distribution of arbitrarily high order. This idea has been exploited by George *et al.* [10] to locate phase boundaries in disordered Ising models, and it is also being dicussed in a recent preprint of Paladin *et al.* [28].

Finally, it is perhaps worth pointing out once more that the equlibrium ensemble approach appears to be well suited to study problems with *correlated* disorder, as is borne out by the general theory of Sec. 2, and by the more specific considerations of Sec. 4. Within the framework of (low order) moment matching schemes at least, correlated disorder appears to be hardly more complicated than uncorrelated disorder. Regarding more conventional approaches, this can — at best — be claimed for correlated disorder of the Gaussian type.

Acknowlegements: The author is indebted to A. Huber for having acquainted him with Morita's ideas. Illuminating discussions with B. Derrida, H. Horner, R. Stinchcombe, J. Vannimenus, and F. Wegner are gratefully acknowledged. It is a pleasure to thank the members of the Instituut voor Theoretische Fysica at K.U. Leuven for the hospitality extended to him, while parts of this paper were being written, and D. Bollé and J. van Mourik for helpful comments.

References

[1] R. Brout, Phys. Rev. **115**, 824 (1959)

[2] J.M. Luck, *Systèmes Désordres Unidimensionels* (Collection Aléa, Saclay, 1992)

[3] B.M. McCoy and T.T. Wu, Phys. Rev. B **56**, ?? (1968)

[4] L.A. Pastur, J. Stat. Phys. **27**, 119 (1982)

[5] M. Mézard, G. Parisi and M.A. Virasoro, *Spin Glass Theory and Beyond* (World Scientific, Singapore, 1989)

[6] T. Morita, J. Math. Phys. **5**, 1401 (1964)

[7] H. Falk, J. Phys. C **9**, L213 (1976)

[8] M.F. Thorpe and D. Beeman, Phys. Rev. B **14**, 188 (1976)

[9] M.F. Thorpe, J. Phys. C **11**, 2983 (1978)

[10] A. Georges, D. Hansel, P. le Doussal, J.M. Maillard and J.P. Bouchaud, J. Physique **47**, 947 (1986)

[11] G. Toulouse and J. Vannimenus, Phys. Rep. **67**, 47 (1980)

[12] G. Sobotta and D. Wagner, Z. Phys. B **33**, 271 (1979)

[13] G. Sobotta and D. Wagner, J. Phys. C **11**, 1467 (1978)

[14] A. Huber, in: *Recent Developments in Condensed Matter Physics*, edited by J.T. Devreese *et al.* (Plenum Press, New York, 1981), p. 138

[15] R. Kühn, PhD Thesis, Kiel (1987)

[16] R. Kühn, D. Grensing, and A. Huber, Z. Phys. B **63**, 447 (1986)

[17] R. Kühn, Phys. Rev. Lett. **73**, 2269 (1994)

[18] J.L. van Hemmen, Phys. Rev. Lett. **49**, 409 (1982)

[19] M. Schwartz, J. Phys. C **18**, 135 (1985)

[20] J. Bricmont and A. Kupiainen, Comm. Math. Phys **116**, 539 (1988)

[21] M. Serva and G. Paladin, Phys. Rev. Lett. **70**, 105 (1993)

[22] R. Kühn, *Equilibrium Ensemble Approach to Disordered Systems II: Thermodynamics and Critical Behaviour of Disordered Ising Models*, in preparation, cited as II in the main text.

[23] R. Mazo, J. Chem. Phys. **39**, 1224 (1963)

[24] E.T. Jaynes, Phys. Rev **106**, 620 (1957)

[25] M. Wortis, Phys. Rev. B **10**, 4665 (1974)

[26] R. Kühn, Z. Phys. B **66**, 167 (1987)

[27] W. Selke, Phys. Rev. Lett. **73**, 3487 (1994); K. Ziegler, *ibid.*, 3488 (1994); J.K. Kim and A. Patrascioiu, *ibid.*, 3489 (1994)

[28] G. Paladin, M. Pasquini, and M. Serva, *Constrained Annealing for Spin–Glasses*, preprint, (1994)