

Interfaces in disordered systems and directed polymer

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Abstract

These informal notes present some mathematical tools useful to compute the static roughness function, by means of Gaussian integrals, the replica trick, and the Gaussian Variational Method (GVM) approximation scheme.

They complement the lecture notes introducing the theoretical framework of the *disordered elastic systems (DES)*, starting from their generic recipe, and then moving to a crash-course on both their statics and dynamics. This minimal description of physical interfaces allows one to focus on the key role of disorder for such emergent structures: how spatial heterogeneities can pin them, and how thermal fluctuations or an increasing external field allow the system to overcome this pinning.

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In these notes we present the three mathematical techniques needed in the computations: the *Gaussian integrals*, the *replica trick*, and the *variational method*. Each of these techniques will first be introduced, and then immediately applied to the Larkin model and to the complete Hamiltonian:

- the Gaussian integrals will be illustrated with a direct computation of $\langle u_q^* u_q \rangle$ of the Larkin model (section 1.5);
- the replica trick will be applied to \mathcal{H} and \mathcal{H}^L in order to average first over disorder and obtain their corresponding effective Hamiltonians $\tilde{\mathcal{H}}$ and $\tilde{\mathcal{H}}^L$ which couple n replicas of the interface (sections 2.4 and 2.5);
- the variational method is finally used to obtain an equation for the optimal quadratic replicated Hamiltonian \mathcal{H}_0 to approximate $\tilde{\mathcal{H}}$, which cannot be exactly solved analytically (sections 3.3 and 3.4).

1 Functional and Gaussian integrals

In the computation of statistical averages of observables, we are confronted with formal discrete sums involving the exponential of $-\beta\mathcal{H}$. In a continuous representation of the system, these discrete sums are promoted to functional integrals. If the Hamiltonian happens to be quadratic in its order parameter, we are in an ideal case for the analytical computation of those averages, since we can use the identities of the *Gaussian integrals*, which include complex and matricial generalizations of the well-known identity $\int_{\mathbb{R}} du \cdot e^{-u^2} = \sqrt{\pi}$. Note that most of the following material comes from [1].

1.1 Discrete and continuous representations in the Fourier space

The notation $\int \mathcal{D}u$, inherited from the formal sum over all the configurations $\sum_{\{s\}}$, is defined via a discrete representation in real space of the system:

$$\int \mathcal{D}u \equiv \prod_i \int_{\mathbb{R}} du_i \quad (1)$$

However, it is more convenient to work in the Fourier space, so we shall translate it into a discrete sum over all the Fourier modes $u_q \in \mathbb{C}$, with the addition of the Jacobian \tilde{J} of this transformation:

$$\prod_i \int_{\mathbb{R}} \frac{du_i}{\pi^{1/2}} \equiv \tilde{J} \sum_{q>0} \int \int_{\mathbb{R}^2} \frac{d\Re(u_q) d\Im(u_q)}{\pi} \quad (2)$$

Since the Fourier transforms of the Hamiltonian and other observables are functions of $\{u_q, u_q^*\}$, we introduce the symbolic notation:

$$\int \int \frac{d\Re(u_q) d\Im(u_q)}{\pi} \equiv \int \int \frac{du_q^* du_q}{2\pi i} \quad (3)$$

where u and u^* are treated as independent variables in the integration, allowing unitary changes of variables $(u, u^*) \rightarrow (\tilde{u}, \tilde{u}^*)$ such that \tilde{u}, \tilde{u}^* are not complex conjugates anymore. Whenever the notation $*$ may be ambiguous in presence of other variables, the complex conjugates of those will be denoted otherwise (e.g. \bar{h}).

Just for the record, the factors $\pi^{1/2}$ and π in (2) are normalization factors, since

$$\begin{cases} \int_{\mathbb{R}} du \cdot e^{-u^2} & = \pi^{1/2} \\ \int \int_{\mathbb{R}^2} d\Re(u) d\Im(u) e^{-|u|^2} & = \pi \end{cases}$$

and the factor $2i$ in the denominator of (3) comes from the Jacobian of the transformation $(\Re(u), \Im(u)) \rightarrow (u, u^*)$:

$$\begin{pmatrix} \Re(u) \\ \Im(u) \end{pmatrix} = \begin{pmatrix} \frac{u+u^*}{2} \\ \frac{u-u^*}{2i} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2i} & -\frac{1}{2i} \end{pmatrix} \begin{pmatrix} u \\ u^* \end{pmatrix} \Rightarrow \text{Jacobian} = \left\| \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2i} & -\frac{1}{2i} \end{pmatrix} \right\| = \frac{1}{2i} \quad (4)$$

We summarize all this with:

$$\int \mathcal{D}u \equiv \prod_i \int du_i \equiv J \prod_{q>0} \int \int du_q^* du_q \quad (5)$$

and consequently, for n replicas of the system:

$$\int \mathcal{D}u_1(\dots)\mathcal{D}u_n \equiv \prod_{a=1}^n \prod_i \int du_{ai} \equiv J \prod_{q>0} \int \int du_1^*(q)du_1(q)(\dots)du_n^*(q)du_n(q) \quad (6)$$

Since we switch from a continuous to a discrete representation of the system (and inversely) in the computation of functional integrals, which were first introduced in *real* space, we recall the relation used for their counterparts in the Fourier space:

$$\frac{1}{2\Omega} \sum_q \equiv \frac{1}{2} \int \frac{d^d q}{(2\pi)^d} \quad (7)$$

where Ω denotes generically the volume of the system in the discrete Fourier space. The factor $1/2$ anticipates the symmetry $-q \leftrightarrow q$ present in quadratic observables (as Hamiltonians or correlation functions, e.g. the roughness) which are functions of the *real* order parameters $u(z)$, in which case we have:

$$\frac{1}{2\Omega} \sum_q = \frac{1}{\Omega} \sum_{q>0} \quad (8)$$

This should typically not be forgotten when one has to take the partial derivative ∂_q , in order to avoid misplaced factors 2...

1.2 Formulary of Gaussian integrals

The Gaussian integrals can all be derived from:

$$\int_{\mathbb{R}} du \cdot e^{-u^2} = \sqrt{\pi} \quad (9)$$

using changes of variables in \mathbb{R} :

$$\int_{\mathbb{R}} du \cdot e^{-au^2} = \sqrt{\frac{\pi}{a}} \quad (a > 0) \quad (10)$$

and then in \mathbb{C} with integrations by parts using the transformations:

$$\int_{\mathbb{C}} \frac{du^* du}{2\pi i} \xrightarrow{[u=x+iy]} \int \int_{\mathbb{R}^2} \frac{dx dy}{\pi} \xrightarrow{[u=\rho \cdot e^{i\theta}]} \frac{1}{\pi} \int_0^{2\pi} d\theta \int_0^\infty d\rho \cdot \rho \quad (11)$$

We thus have for $a \in \mathbb{R}$ the following identities:

$$\int \int \frac{du^* du}{2\pi i} \cdot e^{-au^* u} = \frac{1}{a} \quad (12)$$

$$\int \int \frac{du^* du}{2\pi i} \cdot u \cdot e^{-au^* u} = 0 \quad (13)$$

$$\int \int \frac{du^* du}{2\pi i} \cdot u^* \cdot e^{-au^* u} = 0 \quad (14)$$

$$\int \int \frac{du^* du}{2\pi i} \cdot u^* u \cdot e^{-au^* u} = \frac{1}{a} \int \int \frac{du^* du}{2\pi i} \cdot e^{-au^* u} \quad (15)$$

where the symbolic notation $\int \int du^* du_q$ conveniently allows to consider u, u^* as independent variables. Integrations of *odd* functions of $\{u, u^*\}$ (e.g. $u, u^*, u^2 \cdot u^*, (u^*)^2 \cdot u$, etc.) give zero, as showed by (13) and (14). Integrations of *even* functions of $\{u, u^*\}$ (e.g. $u^* u, u^2 \cdot (u^*)^4$, etc.) bring factors $1/a$ in front of (12) via an integration by parts, as shown by (15).

For M and H $n \times n$ real symmetric and positive definite matrices (e.g. Hamiltonians with an appropriate definition of the zero of energy), the spectral theorem guarantees the existence of an orthonormal vectorial basis in which M and H are diagonal. Using this basis, we can obtain from (10) the following *matricial* Gaussian integral:

$$\int du_1(\dots)du_n \cdot e^{-\sum_{ij} u_i M_{ij} u_j} = \frac{\pi^{n/2}}{(\det M)^{1/2}} \quad (16)$$

and we can extract the coefficients of the inverse matrix of M via:

$$\frac{\int du_1(\dots)du_n \cdot u_k u_l \cdot e^{-\frac{1}{2} \sum_{ij} u_i M_{ij} u_j}}{\int du_1(\dots)du_n \cdot e^{-\frac{1}{2} \sum_{ij} u_i M_{ij} u_j}} = (M^{-1})_{kl} \quad (17)$$

In presence of quadratic and linear terms in the argument of the exponentials, we can complete real or complex ‘matricial squares’ using:

$$\int \frac{du_1(\dots)du_n}{(2\pi)^{n/2}} \cdot e^{-\frac{1}{2} \sum_{ij} u_i M_{ij} u_j + \sum_i b_i u_i} = \frac{e^{\frac{1}{2} \sum_{ij} b_i (M^{-1})_{ij} b_j}}{(\det M)^{1/2}} \quad (18)$$

$$\left(\prod_i \int \frac{du_i^* du_i}{2\pi i} \right) e^{-\sum_{ij} u_i^* H_{ij} u_j + \sum_i (h_i^* u_i + h_i u_i^*)} = \frac{e^{\sum_{ij} h_i^* (H^{-1})_{ij} h_j}}{\det H} \quad (19)$$

The explicit procedure which gives these relations is described in more details in the section 1.4.

1.3 Averages with quadratic Hamiltonians

If a Hamiltonian $\mathcal{H}[u]$ is quadratic in u and diagonal in its Fourier modes q , i.e. of the generic form (in both its representations):

$$\mathcal{H}[u] = \frac{1}{2\Omega} \sum_{\bar{q}} u_{\bar{q}}^* A_{\bar{q}} u_{\bar{q}} = \frac{1}{2} \int \frac{d^d \tilde{q}}{(2\pi)^d} u_{\tilde{q}}^* A_{\tilde{q}} u_{\tilde{q}} \quad (20)$$

with $A_{-\bar{q}} = A_{\bar{q}}$, any average of correlators in Fourier space can be computed using Gaussian identities. The link between those and their functional versions is given thereafter: In a discrete representation:

$$\langle u^*(q_1)u(q_2) \rangle \equiv \frac{\int \mathcal{D}u \cdot u^*(q_1)u(q_2) \cdot \exp \left[-\frac{\beta}{2\Omega} \sum_{\bar{q}} u_{\bar{q}}^* A_{\bar{q}} u_{\bar{q}} \right]}{\int \mathcal{D}u \cdot \exp \left[-\frac{\beta}{2\Omega} \sum_{\bar{q}} u_{\bar{q}}^* A_{\bar{q}} u_{\bar{q}} \right]} = \frac{\Omega \beta^{-1}}{A(q_1)} \cdot \delta_{q_1 q_2} \quad (21)$$

and in its continuous counterpart:

$$\langle u^*(q_1)u(q_2) \rangle \equiv \frac{\int \mathcal{D}u \cdot u^*(q_1)u(q_2) \cdot \exp \left[-\frac{\beta}{2} \int \frac{d^d \tilde{q}}{(2\pi)^d} \cdot u_{\tilde{q}}^* A_{\tilde{q}} u_{\tilde{q}} \right]}{\int \mathcal{D}u \cdot \exp \left[-\frac{\beta}{2} \int \frac{d^d \tilde{q}}{(2\pi)^d} \cdot u_{\tilde{q}}^* A_{\tilde{q}} u_{\tilde{q}} \right]} = \frac{(2\pi)^d \beta^{-1}}{A(q_1)} \cdot \delta(q_1 - q_2) \quad (22)$$

A quadratic *replicated* Hamiltonian, which describes a set of n replicas of the system, also diagonal in its Fourier modes q , is of the generic form:

$$\mathcal{H}[\bar{u}] = \frac{1}{2\Omega} \sum_{\bar{q}} \sum_{a'b'} u_{a'}^*(\bar{q}) G_{a'b'}^{-1}(\bar{q}) u_{b'}(\bar{q}) = \frac{1}{2} \int \frac{d^d \tilde{q}}{(2\pi)^d} \sum_{a'b'} u_{a'}^*(\tilde{q}) G_{a'b'}^{-1}(\tilde{q}) u_{b'}(\tilde{q}) \quad (23)$$

and it follows finally, in a continuous representation of the Fourier modes q :

$$\begin{aligned} \langle u_a^*(q_1)u_b(q_2) \rangle &\equiv \frac{\int \mathcal{D}u_1(\dots)\mathcal{D}u_n \cdot u_a^*(q_1)u_b(q_2) \cdot \exp \left[-\frac{\beta}{2} \int \frac{d^d \tilde{q}}{(2\pi)^d} \cdot \sum_{a'b'} u_{a'}^*(\tilde{q}) G_{a'b'}^{-1}(\tilde{q}) u_{b'}(\tilde{q}) \right]}{\int \mathcal{D}u_1(\dots)\mathcal{D}u_n \cdot \exp \left[-\frac{\beta}{2} \int \frac{d^d \tilde{q}}{(2\pi)^d} \cdot \sum_{a'b'} u_{a'}^*(\tilde{q}) G_{a'b'}^{-1}(\tilde{q}) u_{b'}(\tilde{q}) \right]} \\ &= (2\pi)^d \cdot \beta^{-1} \cdot G_{ab}(q_1) \cdot \delta(q_1 - q_2) \end{aligned} \quad (24)$$

These identities are used throughout the computations of thermal and disorder averages, and when they do not apply, even under a reformulation of the considered averages, we usually cannot pursue exact computations. Note that if \mathcal{H} is diagonal in q , we have δ -functions $\delta(q_1 - q_2)$, even for replicas, whereas different indices a, b for the replicas are authorised and actually allow to extract the coefficients $G_{ab}(q)$.

1.4 To complete a ‘matricial square’

To compute for example thermal averages, we start from a Hamiltonian whose elastic part is quadratic (described by G) and whose disorder part is linear in u, u^* . By completing this ‘matricial square’, we recover a quadratic part through a unitary redefinition of $(u, u^*) \mapsto (\tilde{u}, \tilde{u}^*)$, with an additional term which does not depend on the displacements u, u^* and can thus be taken outside the thermal average. This last term is actually all that will survive to the thermal average.

If G is a Hermitian matrix, $G^\dagger = \bar{G}^T = G$ and we have:

$$\begin{aligned} (u + Gh_1)^\dagger G^{-1} (u + Gh_2) &= u^{*\dagger} G^{-1} u + \bar{h}_1^T \underbrace{G^\dagger G^{-1}} u + u^{*\dagger} \underbrace{G^{-1} G} h_2 + \bar{h}_1^T \underbrace{G^\dagger G^{-1} G} h_2 \\ &\stackrel{[G^\dagger=G]}{=} u^{*\dagger} G^{-1} u + \bar{h}_1^T u + u^{*\dagger} h_2 + \bar{h}_1^T G h_2 \end{aligned} \quad (25)$$

If G is real and symmetric, it is Hermitian and thus:

$$(u + Gh_1)^\dagger = (u^* + G\bar{h}_1)^\top \implies u^{*\top} G^{-1} u + \bar{h}_1^\top u + u^{*\top} h_2 = (u^* + G\bar{h}_1)^\top G^{-1} (u + Gh_2) - \bar{h}_1^\top Gh_2$$

and this last identity becomes in terms of components:

$$\begin{aligned} & \sum_{a'b'} (u_{a'}^* G_{a'b'}^{-1} u_{b'} + \bar{h}_{1a'} \delta_{a'b'} u_{b'} + u_{a'}^* \delta_{a'b'} h_{2b'}) \\ &= (u^* + G\bar{h}_1)^\top G^{-1} (u + Gh_2) - \sum_{a'b'} \bar{h}_{1a'} G_{a'b'} h_{2b'} \end{aligned} \quad (26)$$

1.5 Direct computation of $\langle u_q^* u_q \rangle$ in the Larkin model

To illustrate the use of Gaussian integrals in averages with quadratic Hamiltonians, we compute in this section the structure factor $\langle u_q^* u_q \rangle$ of the Larkin model, for a generic dimension d . Note that the following computations are widely inspired from [1].

The Larkin Hamiltonian, put in its quadratic form, can actually be rewritten as:

$$\mathcal{H}^L [u, f] = \mathcal{H}_{\text{el}} [\tilde{u}] - \frac{1}{2} \int_{(\mathcal{D}_z)_q} \frac{d^d q}{(2\pi)^d} \frac{f_q^* f_q}{cq^2} \quad (27)$$

via the following redefinition of the displacement field:

$$\tilde{u}_q = u_q + \frac{f_q}{cq^2} \quad (28)$$

The second term in the Hamiltonian does not depend on the displacements u or \tilde{u} , so at a given disorder f it is a constant which disappears via the thermal average.

We start by computing the structure factor at fixed disorder f , using the change of variable $(u, u^*) \rightarrow (\tilde{u}, \tilde{u}^*)$ and the linearity of the thermal average:

$$\begin{aligned} \langle u_q^* u_q \rangle_f &\stackrel{(28)}{=} \left\langle \left(\tilde{u}_q^* - \frac{f_q^*}{cq^2} \right) \left(\tilde{u}_q - \frac{f_q}{cq^2} \right) \right\rangle_f \\ &= \underbrace{\langle \tilde{u}_q^* \tilde{u}_q \rangle_f}_{\langle u_q^* u_q \rangle_{f=0}} + \underbrace{\left\langle \frac{f_q^* f_q}{(cq^2)^2} \right\rangle_f}_{\langle \text{cte} \rangle = \text{cte}} - \underbrace{\langle f_q^* u_q + f_q u_q^* \rangle_f}_{=0: \text{lin. in } u, u^*} \\ &= \langle u_q^* u_q \rangle_{f=0} + \frac{f_q^* f_q}{(cq^2)^2} \end{aligned} \quad (29)$$

Then we compute the average over disorder, using again its linearity:

$$\overline{\langle u_q^* u_q \rangle} = \underbrace{\overline{\langle u_q^* u_q \rangle_{f=0}}}_{\text{cte} = \text{cte}} + \frac{\overline{f_q^* f_q}}{(cq^2)^2} = \underbrace{\langle u_q^* u_q \rangle_{f=0}}_{\text{purely thermal}} + \underbrace{\frac{f_q^* f_q}{(cq^2)^2}}_{\text{purely disorder}} \quad (30)$$

The structure factor $\langle u_q^* u_q \rangle$ of the Larkin model splits in two uncoupled contributions: the first one is purely thermal, since it is the genuine structure factor of the case without disorder ($f \equiv 0$); the second one depends exclusively on the disorder. We consider both those terms with the definitions of their respective averages (note the presence of the volume term $(2\pi)^d$, not to be forgotten), and use (22):

$$\begin{aligned} \langle u_q^* u_q \rangle_{f=0} &= \frac{\int \mathcal{D}u \cdot u_q^* u_q \cdot e^{-\frac{\beta}{2} \int \frac{d^d \bar{q}}{(2\pi)^d} \cdot c\bar{q}^2 \cdot u_{\bar{q}}^* u_{\bar{q}}}}{\int \mathcal{D}u \cdot e^{-\frac{\beta}{2} \int \frac{d^d \bar{q}}{(2\pi)^d} \cdot c\bar{q}^2 \cdot u_{\bar{q}}^* u_{\bar{q}}}} = \left(\frac{\beta c q^2}{(2\pi)^d} \right)^{-1} = (2\pi)^d \cdot \frac{T}{c q^2} \\ \overline{f_q^* f_q} &= \frac{\int \mathcal{D}f \cdot f_q^* f_q \cdot e^{-\frac{D-1}{2} \int \frac{d^d \bar{q}}{(2\pi)^d} f_{\bar{q}}^* f_{\bar{q}}}}{\int \mathcal{D}f \cdot e^{-\frac{D-1}{2} \int \frac{d^d \bar{q}}{(2\pi)^d} f_{\bar{q}}^* f_{\bar{q}}}} = \left(\frac{D-1}{(2\pi)^d} \right)^{-1} = (2\pi)^d \cdot D \end{aligned}$$

and we finally obtain:

$$\overline{\langle u_q^* u_q \rangle} = (2\pi)^d \cdot \left(\frac{T}{c q^2} + \frac{D}{(c q^2)^2} \right) \quad (31)$$

The thermal contribution is a propagator in $1/q^2$ and the disorder contribution is in $1/q^4$.

2 The replica theory

To compute analytically the average of an observable \mathcal{O} in a quenched disordered system, we have first to compute its thermal average at fixed disorder, i.e. for a given configuration V of the random potential. The disorder average shall only be computed *afterwards*. Indeed, $\langle \mathcal{O} \rangle_V$ corresponds physically to the expected value of a measurement of \mathcal{O} on a physical sample described by V , whereas $\overline{\langle \mathcal{O} \rangle}$ is the expected value for a self-averaging system, or equivalently for an average over a representative set of samples of different disorder configuration.

Yet we actually never give an explicit form of V , we only impose on it a given statistical distribution, in this case a Gaussian distribution with a standard deviation D . In the Larkin model, the disorder Hamiltonian is linear in $u(z)$ and so it is possible to average explicitly over the displacement field $u(z)$, even with the random variable V , as it is done in the section 1.5. However, for \mathcal{H}_{dis} the $u(z)$ -dependence in the exponential does not allow such an explicit computation. Moreover, for an arbitrary V , the interface is not invariant through a translation in the z direction; this hinders a description in the Fourier space.

So we would like practically to average first over disorder, in order to recover as soon as possible a translation invariance on the interface and to get rid of V , keeping only its relevant parameter, namely the disorder strength D .

The replica theory provides precisely a framework to practically average first over disorder. It has in particular been used by M. Mézard and G. Parisi in the context of the spin-glass theory, and is exposed in their review book [2]. In spin glasses, spins organised in a lattice (for example Ising spins) are coupled via random bonds, of known distribution. The frustration of those randomly coupled spins gives rise to metastability and glassy properties, similarly to the case of our interface.

In brief, the replica trick aims to account for the effect of disorder on a single system by replacing it with n replicas of itself, coupled by an effective Hamiltonian of n displacement fields $\tilde{\mathcal{H}}[u_1, \dots, u_n]$. Quoting [3], those replicas will act ‘as probes exploring the unknown phase space, and sending us important information on the structure of states in it’. Indeed, the valleys of metastability in the complicated energy landscape of a disordered system correspond to clusters of similar configurations. The disorder-averaged couplings of all the possible configurations of an interface should thus encode, somehow, the universal properties of this landscape’s structure.

In this section, we start by introducing in $\langle \mathcal{O} \rangle$ n exact copies of the system via its partition function Z , n being an arbitrary (large) integer. Those *replicas* will act as probes of the system’s behaviour, but they must have disappeared at the end of our computations, taking the limit $n \rightarrow 0$. But before, they will allow the definition of an effective ‘replicated’ Hamiltonian $\tilde{\mathcal{H}}[u_1, \dots, u_n]$, and of its corresponding thermal average, obtained after the disorder average.

The definition of the replicas imposes on $\tilde{\mathcal{H}}$ the structure of a $n \times n$ *hierarchical* matrix, whose properties will then briefly be discussed. Indeed, $\overline{\langle \mathcal{O} \rangle}$ happens to extract the coefficients of the inverse of $\tilde{\mathcal{H}}$, i.e. the coefficients of its Green function (denoted by G in (24)). Inversion formulas for hierarchical matrices are thus needed, and are actually available directly in the limit $n \rightarrow 0$ which interests us. The algebra of such ‘ 0×0 ’ hierarchical matrices has been given in [4]. Thereafter those inversion formulas will be presented, respectively for *replica-symmetric* and *full replica-symmetry-breaking (RSB)* Hamiltonians. The replica trick will be applied to the Larkin model, and the inversion of its effective Hamiltonian $\tilde{\mathcal{H}}^L$ presented as an illustration of a replica-symmetric case.

We will eventually compute explicitly the effective Hamiltonian $\tilde{\mathcal{H}}[\vec{u}]$ of the complete model for $d = m = 1$.

As we will see, the replica trick works under cover of exchanges of limits, and in particular of the analytical continuation from an arbitrary large integer n of replicas to $n \rightarrow 0$. Those can rise a lot of skepticism (and jokes like ‘some consider that the replica theory is a generator of random formulas’), but actually some results obtained via the replicas can be find also by completely different approaches (the cavity method, TAP, cf. [2]), and in some cases a rigorous mathematical justification has been given. In addition to the physical arguments in its favour, this approach thus seems to catch at least some of the physics of the disorder, and that makes it worth the try.

2.1 Introduction of the replica via the partition function: $\frac{1}{Z} = \lim_{n \rightarrow 0} Z^{n-1}$

Practically, the explicit computation of the disorder average is hindered by the presence of disorder both in the numerator and in the partition function in the denominator of the thermal average. In order to bypass

this, we add n exact replicas of the system, using its partition function:

$$\frac{1}{Z} = \lim_{n \rightarrow 0} \frac{Z^n}{Z} = \lim_{n \rightarrow 0} Z^{n-1} \quad (32)$$

which means, for the partition function of the system at equilibrium $Z[V] = \int \mathcal{D}u \cdot e^{-\beta\mathcal{H}[u,V]}$:

$$\begin{aligned} \frac{1}{Z} &= \lim_{n \rightarrow 0} Z^{n-1} = \int \mathcal{D}u_2 \cdot e^{-\beta\mathcal{H}[u_2,V]} \cdot (\dots) \cdot \int \mathcal{D}u_n \cdot e^{-\beta\mathcal{H}[u_n,V]} \\ &= \int \mathcal{D}u_2(\dots)\mathcal{D}u_n \cdot e^{-\beta \sum_{i=2}^n \mathcal{H}[u_i,V]} \end{aligned} \quad (33)$$

For the thermal average of an observable \mathcal{O} , we can thus formally promote the partition function in the denominator as a product of replicas in the numerator:

$$\begin{aligned} \langle \mathcal{O} \rangle &\equiv \frac{1}{Z} \int \mathcal{D}u \cdot \mathcal{O}[u] \cdot e^{-\beta\mathcal{H}[u,V]} = \lim_{n \rightarrow 0} Z^{n-1} \int \mathcal{D}u_1 \cdot \mathcal{O}[u_1] \cdot e^{-\beta\mathcal{H}[u_1,V]} \\ &= \lim_{n \rightarrow 0} \int \mathcal{D}u_1(\dots)\mathcal{D}u_n \cdot \mathcal{O}[u_1] \cdot e^{-\beta \sum_{i=1}^n \mathcal{H}[u_i,V]} \end{aligned} \quad (34)$$

and finally, after the disorder average, we can define an effective Hamiltonian $\tilde{\mathcal{H}}$:

$$\overline{\langle \mathcal{O} \rangle} = \lim_{n \rightarrow 0} \int \mathcal{D}u_1(\dots)\mathcal{D}u_n \cdot \mathcal{O}[u_1] \cdot \overline{\exp\left(-\beta \sum_i \mathcal{H}[u_i, V]\right)} \quad (35)$$

$$\equiv \lim_{n \rightarrow 0} \int \mathcal{D}u_1(\dots)\mathcal{D}u_n \cdot \mathcal{O}[u_1] \cdot \exp\left(-\beta \tilde{\mathcal{H}}[\vec{u}]\right) \quad (36)$$

The replica trick thus allows to formally replace $\overline{\langle \mathcal{O} \rangle}$ with a ‘replicated’ thermal average over an effective Hamiltonian $\tilde{\mathcal{H}}[\vec{u}]$, which a priori couples the replicas. If the disorder Hamiltonian is linear in V , as it is the case in our model, this effective Hamiltonian can be computed explicitly using Gaussian integrals.

The computation of $\overline{\langle \mathcal{O} \rangle}$ is thus available through the inversion of $\tilde{\mathcal{H}}[\vec{u}]$ and the obtention of its Green function. It is exactly possible for the Larkin model, and we obtain indeed the same result as by a direct computation (31). The programme is the following: we have to inverse $\tilde{\mathcal{H}}[\vec{u}]$ and to apply the limit $n \rightarrow 0$: welcome into the realm of the 0×0 hierarchical matrices (!), explored among others by Mézard and Parisi, and briefly presented thereafter.

2.2 Properties of a hierarchical matrix

The replica trick imposes on the effective Hamiltonian the structure of a $n \times n$ *hierarchical matrix*. Indeed, a replicated Hamiltonian must be *symmetrical* in u_q and u_q^* , since $u_q^* = u_{-q}$ and the choice to sum over the Fourier modes q or $-q$ must be irrelevant. Moreover, the choice of the index of the displacement fields in (34) is completely arbitrary, so *each line of a replicated Hamiltonian must be a permutation of the other lines*. By symmetry, each of its column must also be a permutation of the other columns. This constraint actually shortens the number of permutations to the n sequences of coefficients which respect this symmetry, even though there is still some freedom in their possible arrangement.

A generic $n \times n$ hierarchical matrix \hat{G} and its corresponding inverse matrix \hat{G}^{-1} , also hierarchical, are symmetrical and can be written:

$$\hat{G} \equiv \begin{pmatrix} \tilde{G} & & G_{a \neq b} \\ & \ddots & \\ G_{a \neq b} & & \tilde{G} \end{pmatrix} \iff \hat{G}^{-1} \equiv \begin{pmatrix} \tilde{G}^{-1} & & G_{a \neq b}^{-1} \\ & \ddots & \\ G_{a \neq b}^{-1} & & \tilde{G}^{-1} \end{pmatrix} \quad (37)$$

where $\tilde{G} = G_{aa}$ and $\tilde{G}^{-1} = G_{aa}^{-1} \quad \forall a$. The exponent -1 is used exclusively in relation with the inverse matrix \hat{G}^{-1} , and shall not be mistaken with the negative power exponent of a scalar (e.g. $G_{aa}^{-1} \neq (G_{aa})^{-1}$). The tilde refers to the diagonal elements of the matrix.

Since the different coefficients of a hierarchical matrix are repeated in each line and in each column, the knowledge of a single line or column is enough to construct the whole matrix. One can thus choose as reference the sequence in which the coefficients are classified monotonously, and put it in the first line of

the matrix. This property allows the definition of the *connected* part of these matrices, i.e. the sum of the coefficients on any line or column:

$$G_c = \sum_a G_{ab} = \sum_b G_{ab} \iff G_c^{-1} = \sum_a G_{ab}^{-1} = \sum_b G_{ab}^{-1} \quad (38)$$

Those connected parts actually satisfy $G_c \cdot G_c^{-1} = 1$, by definition of an inverse matrix:

$$G_c \cdot G_c^{-1} = \left(\sum_a G_{ab} \right) \left(\sum_b G_{ba'}^{-1} \right) = \sum_a \underbrace{\left(\sum_b G_{ab} G_{ba'}^{-1} \right)}_{\delta_{aa'}} = 1 \iff G_c = \frac{1}{G_c^{-1}} \quad (39)$$

The simplest case of a hierarchical matrix is the *replica-symmetric* Ansatz, in which all the off-diagonal coefficients of the matrix are equal:

$$G_{a \neq b} = G \quad \forall a, b \implies \hat{G} = \begin{pmatrix} \tilde{G} & G \\ & \ddots \\ G & \tilde{G} \end{pmatrix} \quad (40)$$

If the off-diagonal terms count at least two different values $\{g_0, \dots, g_k\}$, we have a *replica-symmetry breaking (RSB)* Ansatz. The integer k corresponds to the number of such breakings, but for a full description of the matrix it must be coupled to the weight of each new coefficient g_j , as illustrated by FIG 1.

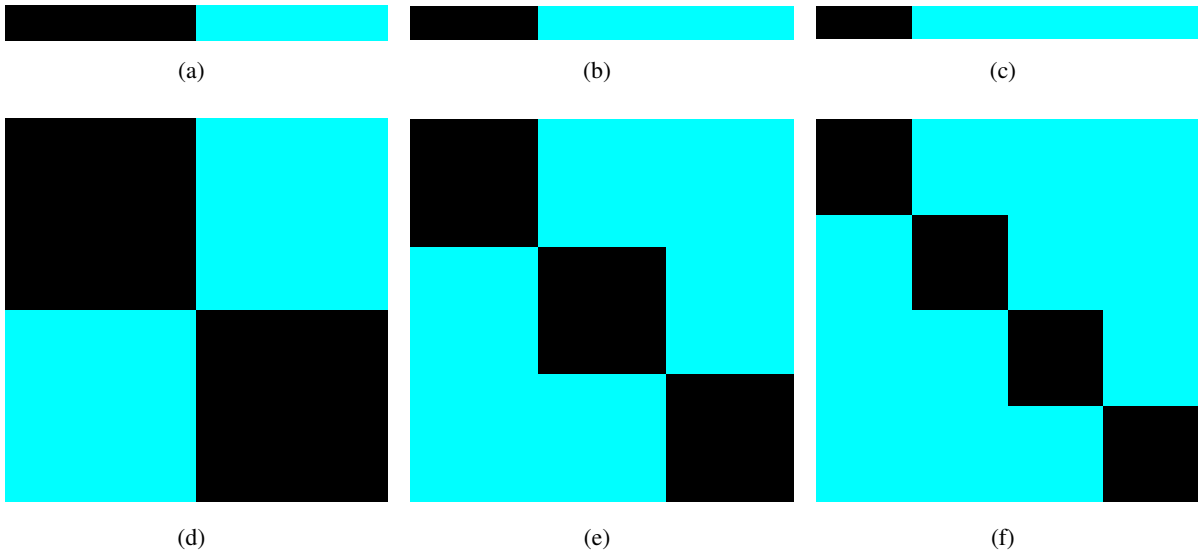


Figure 1: Examples of hierarchical matrices with one symmetry-breaking ($k = 1$); (a)-(c) correspond to the reference sequence of those matrices, the two colors illustrating the two different values of the coefficients. The distribution of those values dictates the structure of the whole matrix; the black zones thus occupy respectively one half (a), one third (b) and one quarter (c) of the reference sequence.

By construction, a $n \times n$ hierarchical matrix can have at most $k = n$ symmetry-breaking. But since n is itself an arbitrary integer in the replica trick, it can as well be taken equal to a power of two $n = 2^m$ with $m \in \mathbb{N}$, which allows to completely fragment the matrix, as illustrated in FIG 2. Taking $m \rightarrow \infty$, the monotonous sequence of coefficients on the first line of the matrix is more adequately described by a monotonous function $G(u)$, depending on a mapping parameter $u \in [0, 1]$:

$$\{g_0, \dots, g_k\} \mapsto G(u) \quad u \in [0, 1] \quad (41)$$

We can thus define a *full RSB* hierarchical matrix with:

$$\hat{G} = \begin{pmatrix} \tilde{G} & G(u) \\ & \ddots \\ G(u) & \tilde{G} \end{pmatrix} \quad \text{with } u \in [0, 1] \quad (42)$$

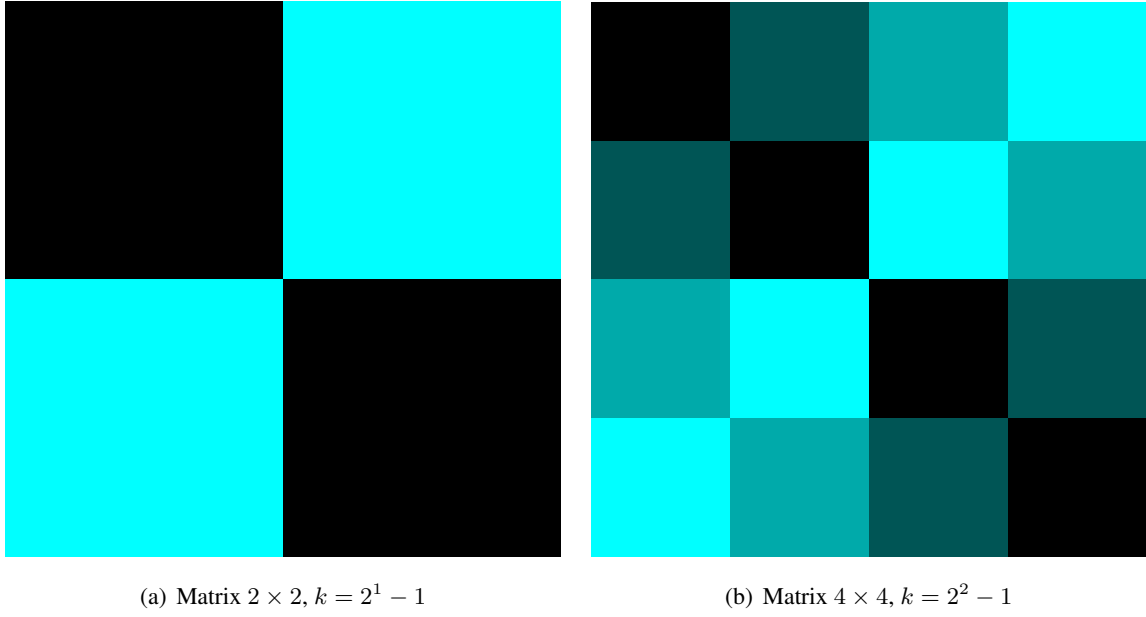


Figure 2: Examples of hierarchical matrices of $n \times n$ blocks, with increasing integer k of replica-symmetry breaking. Each shade of color from black to cyan corresponds to a different value for the coefficients of the matrices. See also Fig. 3.

since the first line described by $G(u)$ determines the whole matrix, as illustrated by FIG 3. The full-RSB Ansatz is actually the most generic description of a hierarchical matrix, since the replica-symmetric and k-RSB Ansätze can be recovered using step-functions for $G(u)$.

The peculiar symmetries of hierarchical matrices allow to determine generic inversion formulas, once the first line of the matrix is given, directly in the limit $n \rightarrow 0$. Those formulas are given in the next section, for the replica-symmetric and the full-RSB cases.

2.3 Inversion formulas of hierarchical matrices in the limit $n \rightarrow 0$

Thereafter the inversion formulas in $n \rightarrow 0$ are given for the replica-symmetric and the full-RSB cases. In the next section the effective Hamiltonian of the Larkin model $\tilde{\mathcal{H}}^L$ and of the complete model $\tilde{\mathcal{H}}$ will be computed and discussed, in relation with the possible obtention of their corresponding Green functions.

From now on, the Hamiltonians will be parametrized by $\hat{G}^{-1}(q)$ and their corresponding Green functions by $\hat{G}(q)$ as generic hierarchical matrices, as in (23). So the thermal average (36) becomes for the structure factor (cf. (24)):

$$\overline{\langle u_q^* u_q \rangle} = \lim_{n \rightarrow 0} \langle u_q^* u_q \rangle_{\tilde{\mathcal{H}}} = (2\pi)^d \cdot T \cdot \lim_{n \rightarrow 0} \tilde{G}(q) \quad (43)$$

2.3.1 Inversion of a replica symmetric Ansatz for $n \rightarrow 0$

For a generic replica-symmetric matrix \hat{G}^{-1} , we have

$$\hat{G}^{-1} = \begin{pmatrix} \tilde{G}^{-1} & & G^{-1} \\ & \ddots & \\ G^{-1} & & \tilde{G}^{-1} \end{pmatrix} \implies \hat{G} = \begin{pmatrix} \tilde{G} & & G \\ & \ddots & \\ G & & \tilde{G} \end{pmatrix}$$

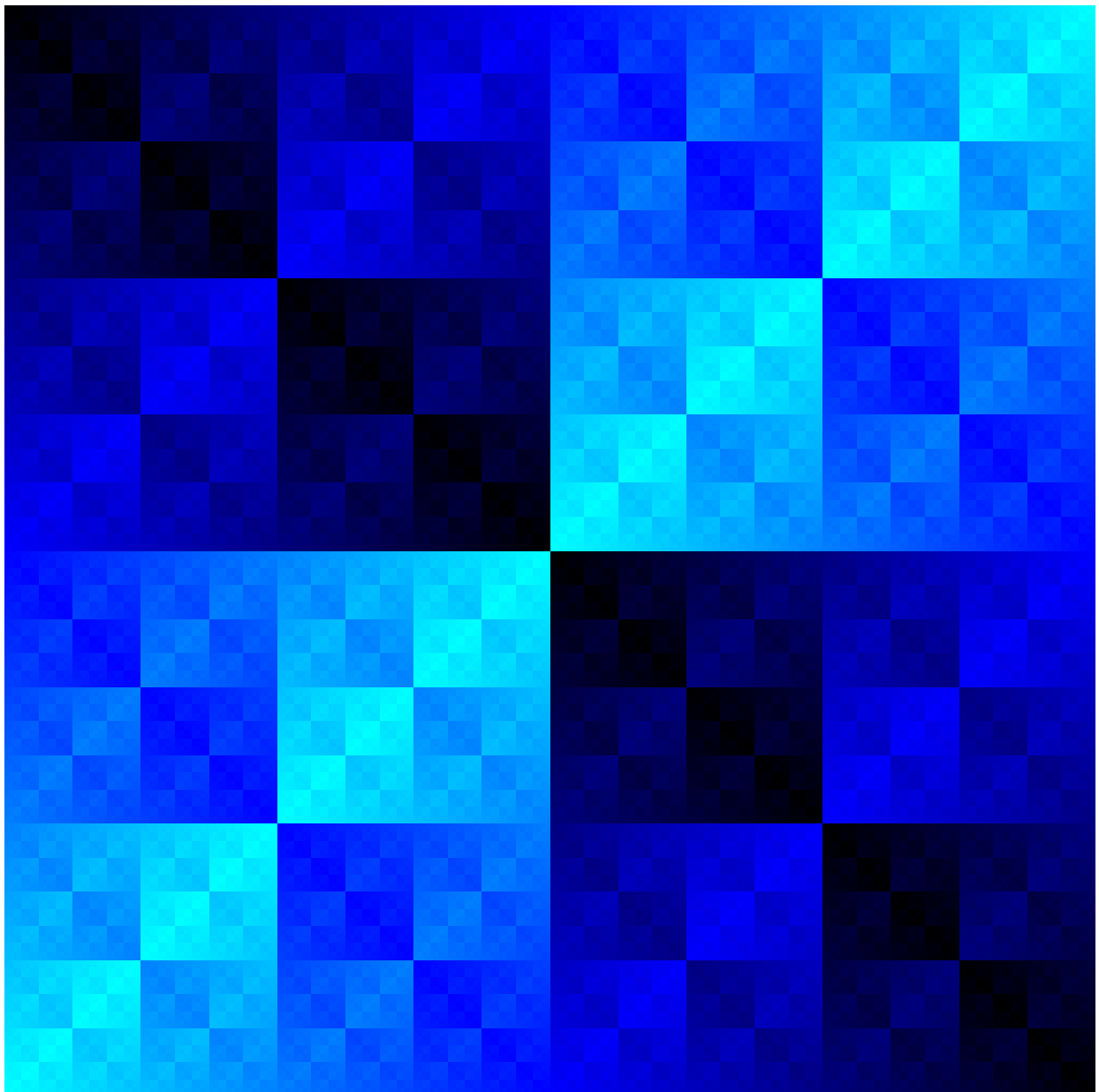
and in the limit $n \rightarrow 0$

$$G_c^{-1} \equiv \tilde{G}^{-1} - G^{-1}, \quad G_c \equiv \tilde{G} - G \\ G_c \cdot G_c^{-1} = 1, \quad G = -\frac{G^{-1}}{(G_c^{-1})^2}, \quad \tilde{G} = \frac{\tilde{G}^{-1} - 2G^{-1}}{(G_c^{-1})^2} \quad (44)$$

These relations can be obtained either by constructing and using an orthonormal vectorial basis in which the $n \times n$ matrix \hat{G}^{-1} becomes diagonal, and finally make n tend to 0, or by solving explicitly the equations which define the inverse of the matrix $\sum_b G_{ab} G_{bc}^{-1} = \delta_{ac}$ directly in the limit $n \rightarrow 0$.



(a) Blend representation of $G(u)$ $u \in [0, 1]$: each shade of color accounts for a possibly different value of the matrix's coefficients.



(b) Full RSB hierarchical matrix

Figure 3: Illustration of a full RSB hierarchical matrix using a blend representation (in fact a completely fragmented 256×256 block matrix with $k = 2^8 - 1$, which goes beyond the resolution of the impression).

2.3.2 Full Replica Symmetry Breaking (RSB) for $n \rightarrow 0$

The full-RSB inversion formulas are given in [5]. Thereafter they have been adapted to the following definition of full-RSB hierarchical matrices:

$$\widehat{G}^{-1}(q) = \begin{pmatrix} G_c^{-1} - \tilde{\sigma} & & -\sigma(u) \\ & \ddots & \\ -\sigma(u) & & G_c^{-1} - \tilde{\sigma} \end{pmatrix} \implies \widehat{G}(q) = \begin{pmatrix} \widetilde{G}(q) & & G(q, u) \\ & \ddots & \\ G(q, u) & & \widetilde{G}(q) \end{pmatrix}$$

$\sigma(u)$ being defined as a monotonous function on the dense interval $[0, 1]$, the discrete sums of matricial operations are replaced by integrals. With the definition:

$$[\sigma](v) \equiv v \cdot \sigma(v) - \int_0^v dw \cdot \sigma(w) \quad (45)$$

we thus have:

$$G(u) = \frac{1}{G_c^{-1}} \left(\frac{1}{u} \cdot \frac{[\sigma](u)}{G_c^{-1} + [\sigma](u)} + \int_0^u \frac{dv}{v^2} \frac{[\sigma](v)}{G_c^{-1} + [\sigma](v)} + \frac{\sigma(0)}{G_c^{-1}} \right) \quad (46)$$

$$\widetilde{G} = \frac{1}{G_c^{-1}} \left(1 + \int_0^1 \frac{dv}{v^2} \cdot \frac{[\sigma](v)}{G_c^{-1} + [\sigma](v)} + \frac{\sigma(0)}{G_c^{-1}} \right) \quad (47)$$

$$\widetilde{G} - G(u) = \frac{1}{u} \cdot \frac{1}{G_c^{-1} + [\sigma](u)} - \int_u^1 \frac{dv}{v^2} \cdot \frac{1}{G_c^{-1} + [\sigma](v)} \quad (48)$$

$$\widetilde{G} - G(u) = \frac{1}{G_c^{-1} + [\sigma](1)} + \int_u^1 dv \cdot \frac{\sigma'(v)}{(G_c^{-1} + [\sigma](v))^2} \quad (49)$$

2.4 Effective Hamiltonian for the Larkin model $\widetilde{\mathcal{H}}^L$

In this section we apply the replica trick to the Larkin Hamiltonian \mathcal{H}^L , in order to obtain its corresponding effective Hamiltonian $\widetilde{\mathcal{H}}^L$ after averaging over disorder. Thereafter we give all the details of this computation, as a concrete illustration of the replica trick.

We have to compute here:

$$\overline{\exp \left(-\beta \sum_i \mathcal{H}^L [u_i, f] \right)} = \exp \left(-\beta \sum_i \mathcal{H}_{\text{el}} [u_i] \right) \cdot \overline{\exp \left(-\beta \sum_i \mathcal{H}_{\text{dis}}^L [u_i, f] \right)} \quad (50)$$

Using the definition of the disorder average, the second term requires to complete the following ‘square’ in the argument of the exponential:

$$\begin{aligned} & -\beta \sum_i \mathcal{H}_{\text{dis}} [u_i, f] - \frac{D^{-1}}{2} \int \frac{d^d q}{(2\pi)^d} \cdot f_q^* f_q \\ &= -\frac{\beta}{2} \int \frac{d^d q}{(2\pi)^d} \sum_i (f_q u_i^*(q) + f_q^* u_i(q)) - \frac{D^{-1}}{2} \int \frac{d^d q}{(2\pi)^d} \cdot f_q^* f_q \\ &= -\frac{D^{-1}}{2} \int \frac{d^d q}{(2\pi)^d} \left[\underbrace{\left(f_q^* + \beta D \sum_i u_i^*(q) \right)}_{\equiv \tilde{f}_q^*} \underbrace{\left(f_q + \beta D \sum_i u_i(q) \right)}_{\equiv \tilde{f}_q} - \beta^2 D^2 \left(\sum_i u_i^*(q) \right) \left(\sum_i u_i(q) \right) \right] \end{aligned} \quad (51)$$

Since the Jacobian of the transformation $f_q \rightarrow \tilde{f}_q \equiv f_q + \beta D \sum_i u_i(q)$ is equal to one, we have:

$$\int \mathcal{D}f \longrightarrow \int \mathcal{D}\tilde{f}$$

and consequently:

$$\overline{\exp \left(-\beta \sum_i \mathcal{H}^L [u_i, f] \right)} = e^{\frac{\beta^2}{2} \int \frac{d^d q}{(2\pi)^d} (\sum_i u_i^*(q)) (\sum_i u_i(q))} \cdot \underbrace{\frac{1}{C} \int \mathcal{D}\tilde{f} \cdot e^{-\frac{D^{-1}}{2} \int \frac{d^d q}{(2\pi)^d} \cdot \tilde{f}_q^* \tilde{f}_q}}_{=1} \quad (52)$$

Combining (50) and (52), we obtain the effective Hamiltonian for the Larkin model:

$$\tilde{\mathcal{H}}^L[\vec{u}] = \frac{1}{2} \int \frac{d^d q}{(2\pi)^d} \cdot \vec{u}_q^{*\top} \left(cq^2 \mathbb{I}_n - \beta D \begin{pmatrix} 1 & - & 1 \\ | & \backslash & | \\ 1 & - & 1 \end{pmatrix} \right) \vec{u}_q \quad (53)$$

where \mathbb{I}_n is the $n \times n$ identity matrix.

This Hamiltonian is clearly replica-symmetric, and using the inversion formulas (44):

$$\begin{cases} \tilde{G}^{-1} = cq^2 - \beta D \\ G^{-1} = -\beta D \\ G_c^{-1} = cq^2 \end{cases} \xrightarrow{(44)} \begin{cases} G_c = \frac{1}{cq^2} \\ G = \frac{\beta D}{(cq^2)^2} \\ \tilde{G} = \frac{1}{cq^2} + \frac{\beta D}{(cq^2)^2} \end{cases} \quad (54)$$

which gives eventually, using (43), the same result as obtained previously by a direct computation of the averages (cf. (31)):

$$\overline{\langle u_q^* u_q \rangle} = (2\pi)^d \cdot \left(\frac{T}{cq^2} + \frac{D}{(cq^2)^2} \right) \quad (55)$$

We may briefly comment the structure of (53):

- If there is no disorder, $D = 0$ and $\tilde{\mathcal{H}}^L$ is simply a replicated elastic Hamiltonian, in which the replicas are uncoupled.
- The factor D is inherited by the linearity of $\mathcal{H}_{\text{dis}}^L$ in V .
- The matrix of 1 describes an equivalent coupling between the replicas. This can be interpreted as following: in a perturbative approach, the averaged effect of disorder exhibits an equivalence between all the possible configurations u of a weakly distorted interface, even in the most disparate pair of configurations. This does not seem to account for the presence of metastability in the system.
- The disorder contribution does not depend on q , so the equivalence between the replicas in Fourier space appears also in real space.

2.5 Effective Hamiltonian for the complete model $\tilde{\mathcal{H}}$

In this section we finally apply the replica trick to the Hamiltonian \mathcal{H} of the complete DES model. After averaging over disorder, it actually reduces to the following effective Hamiltonian which couples the replicas:

$$\tilde{\mathcal{H}}[\vec{u}] = \frac{1}{2} \int \frac{dq}{2\pi} \cdot cq^2 \sum_a u_a^*(q) u_a(q) - \frac{\beta D}{2} \int_{\mathbb{R}} \frac{d\lambda}{2\pi} \cdot e^{-\lambda^2 \xi^2} \int dz \cdot \sum_{ab} e^{i\lambda(u_a(z) - u_b(z))} \quad (56)$$

Because of the term $\sum_{ab} \int dz \cdot e^{i\lambda(u_a(z) - u_b(z))}$, we do not know how to reformulate $\tilde{\mathcal{H}}$ in a quadratic form in Fourier space, such as (23). Consequently we have not access to the diagonal term $\tilde{G}(q)$ of its Green function, and we cannot compute thermal averages $\langle \mathcal{O} \rangle_{\tilde{\mathcal{H}}}$ using (43). In particular, we cannot compute the structure factor $\overline{\langle u_q^* u_q \rangle}$ and its corresponding roughness $B(r)$.

In the next section, we will thus try a variational method to construct the best replicated quadratic Hamiltonian \mathcal{H}_0 , whose Green function will be used to approximate $\tilde{\mathcal{H}}$ in the computation of the average (43):

$$\overline{\langle u_q^* u_q \rangle} \approx \lim_{n \rightarrow 0} \langle u_q^* u_q \rangle_0 = (2\pi)^d \cdot T \cdot \lim_{n \rightarrow 0} \tilde{G}(q) \quad (57)$$

The alternative of a perturbative approach leads to the Larkin model, which is indeed exactly solvable, but such a perturbative expansion is incorrect in $d = 1$. However, even for higher dimensions, it is valid only in the restricted regime of small distortions of the interface, whereas a variational approximation shall not be limited to such a regime.

Thereafter we briefly comment the structure of (56), in comparison with \mathcal{H}^L :

- If there is no disorder, $D = 0$ and $\tilde{\mathcal{H}}$ is again simply a replicated elastic Hamiltonian, in which the replicas are uncoupled.

- The averaged disorder contribution is again proportional to D , inherited from the linearity in V of the physical Hamiltonian \mathcal{H} .
- Unlike the Larkin model, the averaged effect of disorder exhibits a complex coupling of the replicas. In fact, $\int dz \cdot e^{i\lambda(u_a(z)-u_b(z))}$ somehow reminds of a distance between two replicas of the system, as illustrated by FIG 4. Indeed, $\int dz$ sums over all the relative displacements between two possible configurations u_a and u_b for a given λ (Fourier mode in the x direction), and each such pair of replicas contributes to the effective Hamiltonian via \sum_{ab} . This may account for the presence of metastability in the system.

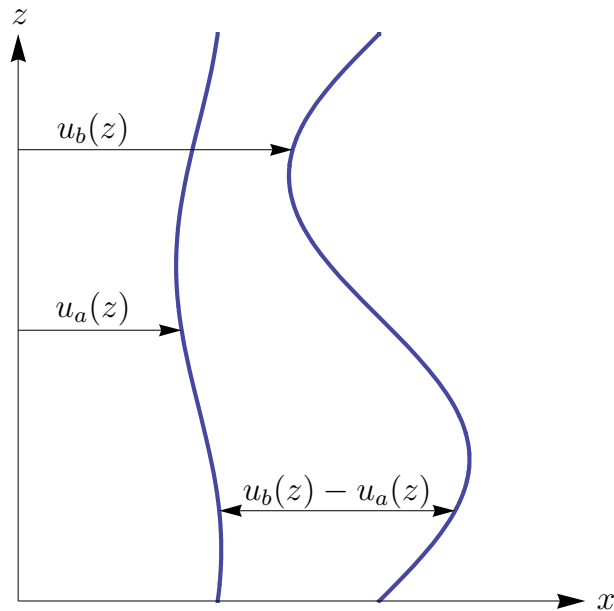


Figure 4: ‘Distance’ between two configurations u_a and u_b .

3 The variational method

Let us suppose that we have to deal with a Hamiltonian \mathcal{H} which cannot be easily manipulated to compute analytically thermal averages of observables. This means usually that the Hamiltonian is not quadratic, in which case the well-known Gaussian integrals do not apply. The replica trick and the disorder average applied on our model has left us precisely with such a Hamiltonian, by providing us with $\tilde{\mathcal{H}}$ in (56).

If there is no other mathematical trick to compute exact results, we will have to try approximation methods. For example a perturbative approach could provide accurate results, but only in the specific regime where the expansion parameter is small enough. For an interface, the Larkin model is indeed valid only for $|u(z)| \ll \xi$, at least for $d > 1$.

The variational method, based on the Bogoliubov inequality, is a recipe to construct a Hamiltonian \mathcal{H}_0 (for our purpose quadratic, thus manipulable), such that its Boltzmann weight $e^{-\beta\mathcal{H}_0}/Z_0$ is the best approximation to its exact counterpart $e^{-\beta\mathcal{H}}/Z$, in the sense that it has a ‘variational’ free energy \mathcal{F}_{var} as close as possible to the exact free energy \mathcal{F} of the system. Practically, this procedure provides a *saddle point equation* for the trial Hamiltonian’s parameters. If one manages to find solutions of this equation, it is then possible to make \mathcal{H}_0 explicit, and to approximate $\langle \mathcal{O} \rangle \approx \langle \mathcal{O} \rangle_0$, where:

$$\langle \mathcal{O} \rangle \equiv \frac{1}{Z} \int \mathcal{D}u \cdot \mathcal{O}[u] \cdot e^{-\beta\mathcal{H}[u]} = \frac{\int \mathcal{D}u \cdot \mathcal{O}[u] \cdot e^{-\beta\mathcal{H}[u]}}{\int \mathcal{D}u \cdot e^{-\beta\mathcal{H}[u]}} \quad (58)$$

$$\langle \mathcal{O} \rangle_0 \equiv \frac{1}{Z_0} \int \mathcal{D}u \cdot \mathcal{O}[u] \cdot e^{-\beta\mathcal{H}_0[u]} = \frac{\int \mathcal{D}u \cdot \mathcal{O}[u] \cdot e^{-\beta\mathcal{H}_0[u]}}{\int \mathcal{D}u \cdot e^{-\beta\mathcal{H}_0[u]}} \quad (59)$$

In this section, we first present the *Bogoliubov inequality*, which provides the free energy criterion for the optimization of a given trial Hamiltonian \mathcal{H}_0 . Then we describe generically the different steps of the variational method and apply it to a replicated elastic disorder system, in order to obtain its generic saddle point equation. We eventually consider the particular case of our model, by making explicit the content of $\tilde{\mathcal{H}}_{\text{dis}}$ in the saddle point equation.

In the next chapter, we will try as solutions of this saddle point equation a replica-symmetric and a full replica-symmetry-breaking Ansatz for \mathcal{H}_0 , and compute their respective roughness.

3.1 The Bogoliubov inequality

The (Gibbs-)Bogoliubov inequality states that the free energy \mathcal{F} of a system is minimum at equilibrium, i.e. when the system is described by its canonical Boltzmann weight $e^{-\beta\mathcal{H}}/Z$:

$$\mathcal{F} = \langle \mathcal{H} \rangle - TS \leq \langle \mathcal{H} \rangle_0 - TS_0 \equiv \mathcal{F}_{\text{var}} \quad (60)$$

where S and S_0 are respectively the Boltzmann entropy of \mathcal{H} and \mathcal{H}_0 , and T the temperature, as usual. Alternatively, the free energy of a system is given by its partition function via: $\mathcal{F} = -T \log Z$. In fact, since the exact free energy of the system described by \mathcal{H}_0 is $\mathcal{F}_0 = \langle \mathcal{H}_0 \rangle_0 - TS_0$ and one can trivially write $\mathcal{H} = (\mathcal{H} - \mathcal{H}_0) + \mathcal{H}_0$, we can recover the usual formulation of the Bogoliubov inequality:

$$\mathcal{F} \leq \langle \mathcal{H} - \mathcal{H}_0 \rangle_0 + \mathcal{F}_0 \equiv \mathcal{F}_{\text{var}} \quad (61)$$

This relation can be viewed as a consequence of the convexity of the exponential present in the canonical Boltzmann weight. Indeed, for any function $g(x)$ such that

$$\partial_x g(x), \partial_x^2 g(x) \geq 0 \quad \forall x \in [a, b] \subset \mathbb{R}$$

we can write ($\langle \cdot \rangle$ denotes the average over $[a, b]$):

$$\langle g(x) \rangle \geq g(\langle x \rangle) \quad (62)$$

This applies in particular to the exponential of any real scalar function f :

$$\langle \exp(f) \rangle \geq \exp(\langle f \rangle) \quad (63)$$

Using (63) we can obtain the Bogoliubov inequality by comparing the partition functions Z and Z_0 , defined respectively by the classical Hamiltonians \mathcal{H} and \mathcal{H}_0 (thereafter $\sum_{\{\mathbf{s}\}}$ denotes the sum over all the configurations as in an Ising formalism):

$$\begin{aligned} \frac{Z}{Z_0} &= \frac{\sum_{\{\mathbf{s}\}} e^{-\beta\mathcal{H}(\{\mathbf{s}\})}}{\sum_{\{\mathbf{s}\}} e^{-\beta\mathcal{H}_0(\{\mathbf{s}\})}} = \frac{\sum_{\{\mathbf{s}\}} e^{-\beta(\mathcal{H}-\mathcal{H}_0)} e^{-\beta\mathcal{H}_0}}{Z_0} = \sum_{\{\mathbf{s}\}} e^{-\beta(\mathcal{H}-\mathcal{H}_0)} \cdot \frac{e^{-\beta\mathcal{H}_0}}{Z_0} \\ &\equiv \left\langle e^{-\beta(\mathcal{H}-\mathcal{H}_0)} \right\rangle_0 \stackrel{(63)}{\geq} e^{-\beta\langle \mathcal{H}-\mathcal{H}_0 \rangle_0} \iff \frac{Z}{Z_0} \geq e^{-\beta\langle \mathcal{H}-\mathcal{H}_0 \rangle_0} \end{aligned} \quad (64)$$

Taking the logarithm to obtain the free energies \mathcal{F} and \mathcal{F}_0 , it follows that:

$$\log Z - \log Z_0 \geq -\beta \langle \mathcal{H} - \mathcal{H}_0 \rangle_0 \iff \underbrace{-\beta^{-1} \log Z}_{\mathcal{F}} \leq \langle \mathcal{H} - \mathcal{H}_0 \rangle_0 \underbrace{-\beta^{-1} \log Z_0}_{\mathcal{F}_0} \quad (65)$$

which is precisely the inequality (61) we were looking for.

Just for the record, the Bogoliubov inequality is valid even if the Hamiltonians \mathcal{H} and \mathcal{H}_0 are operators, as in quantum systems. In general operators do *not* commute, so one cannot simply state that $e^{-\beta\mathcal{H}} = e^{-\beta(\mathcal{H}-\mathcal{H}_0)}e^{-\beta\mathcal{H}_0}$, and (63) has to be proven for f being a matrix.

3.2 Description of the variational method

We would like to solve the exact Hamiltonian \mathcal{H} of a system, i.e. to manage to compute its partition function Z and its free energy $\mathcal{F} = -\beta^{-1} \log Z$, aiming to compute the thermal average of observables $\langle \mathcal{O} \rangle$ (typically correlation functions).

If this is not possible analytically, we can replace the exact Boltzmann weight $\rho = \frac{e^{-\beta\mathcal{H}}}{Z}$ with $\rho_0 = \frac{e^{-\beta\mathcal{H}_0}}{Z_0}$, where \mathcal{H}_0 can be solved (i.e. Z_0 and \mathcal{F}_0 can be computed). The Bogoliubov inequality (61) guarantees that the exact free energy of the system is the lower limit for any variational free energy $\mathcal{F}_{\text{var}} \equiv \langle \mathcal{H} \rangle_0 - TS_0 = \langle \mathcal{H} - \mathcal{H}_0 \rangle_0 + \mathcal{F}_0$. One may hope that the closer those free energies are, the best the approximation $\langle \mathcal{O} \rangle \approx \langle \mathcal{O} \rangle_0$ physically is. Thus the optimal \mathcal{H}_0 is obtained by minimizing \mathcal{F}_{var} .

The generic procedure of the variational method is as follows:

- we define a trial Hamiltonian \mathcal{H}_0 which depends on a set of parameters $\{\lambda_i\}$;
- we make explicit the corresponding \mathcal{F}_{var} as a function of $\{\lambda_i\}$;
- we minimize \mathcal{F}_{var} in respect of $\{\lambda_i\}$, by applying the condition

$$\frac{\partial \mathcal{F}_{\text{var}} \left\{ \tilde{\lambda}_i \right\}}{\partial \lambda_i} = 0 \quad \forall i \quad (66)$$

(one can possibly use Lagrange multipliers to constrain the form of \mathcal{H}_0 at this stage);

- we solve the saddle point equation thus obtained for the $\{\tilde{\lambda}_i\}$;
- we fix the optimal form of \mathcal{H}_0 given by the $\{\tilde{\lambda}_i\}$, and uses it to compute the corresponding averages $\langle \mathcal{O} \rangle_0$.

For completeness one should verify that the solutions of (66) correspond indeed to minima of \mathcal{F}_{var} , since the saddle point equation picks up its maxima as well, if there are any. In principle the Hessian matrix $\left\{ \frac{\partial^2 \mathcal{F}_{\text{var}}}{\partial \lambda_i \partial \lambda_j} \right\}$ is needed to study the stability of those solutions, and to discriminate between the minima and the maxima of \mathcal{F}_{var} . Or we could use our intuition of the physics of the problem to check the plausibility of the available solutions. If there is only a few of them, the comparison of their respective variational free energies eventually closes the argument. However one has to remember that this variational approximation is not controlled, and that it can possibly produce non-physical artefacts, especially if \mathcal{H} and \mathcal{H}_0 differ too much.

3.3 Quadratic Ansatz \mathcal{H}_0 for a disordered elastic system with replicas

In this section, we aim to obtain the generic saddle point equation for the optimal approximation of a disordered elastic system with replicas, considering a trial quadratic Hamiltonian \mathcal{H}_0 parametrized by $\hat{G}^{-1}(q)$ (as in (23)):

$$\mathcal{H}_0[\vec{u}] = \frac{1}{2} \int \frac{d^d q}{(2\pi)^d} \sum_{ab} u_a^*(q) G_{ab}^{-1}(q) u_b(q) \quad (67)$$

After the introduction of the replicas and the disorder average, a generic disordered elastic system is described by an effective Hamiltonian $\tilde{\mathcal{H}}$ such as:

$$\tilde{\mathcal{H}}[\vec{u}] = \tilde{\mathcal{H}}_{\text{el}}[\vec{u}] + \tilde{\mathcal{H}}_{\text{dis}}[\vec{u}] = \frac{1}{2} \int \frac{d^d q}{(2\pi)^d} \cdot c(q) \cdot \sum_a u_a^*(q) u_a(q) + \tilde{\mathcal{H}}_{\text{dis}}[\vec{u}] \quad (68)$$

where $c(q)$ is the energy per Fourier mode q for each replica u_a . $\tilde{\mathcal{H}}_{\text{dis}}$ is left generic since it depends on the specific model for disorder which is considered.

The details of the computation are given thereafter, but at the end we actually obtain the following equation for the optimal \mathcal{H}_0 coefficients:

$$G_{ab}^{-1}(q) = c(q) \cdot \delta_{ab} + \frac{1}{T} \frac{\partial}{\partial G_{ab}(q)} \left\langle \tilde{\mathcal{H}}_{\text{dis}} \right\rangle_0 \quad (69)$$

If there is no disorder, $\left\langle \tilde{\mathcal{H}}_{\text{dis}} \right\rangle_0 = 0$ and $G_{ab}^{-1}(q) = c(q) \cdot \delta_{ab}$: we have just found out that the best quadratic approximation of an elastic Hamiltonian (which is already quadratic) is trivially itself.

In our model, the elastic forces are short ranged and $c(q) = cq^2$. Moreover, the disorder is supposed random-bond and uncorrelated; since \mathcal{H}_{dis} is purely local in z by construction, $\partial_{G_{ab}(q)} \left\langle \tilde{\mathcal{H}}_{\text{dis}} \right\rangle_0$ shall *not* depend on q anymore, as it is indeed the case. All the q dependence of $G_{ab}^{-1}(q)$ is inherited from the elastic part of the Hamiltonian. We thus have:

$$G_{ab}^{-1}(q) = cq^2 \delta_{ab} - \sigma_{ab} \quad \text{with} \quad \sigma_{ab} \equiv -\frac{1}{T} \frac{\partial}{\partial G_{ab}} \left\langle \tilde{\mathcal{H}}_{\text{dis}} \right\rangle_0 \quad (70)$$

If there is disorder, (70) is highly non-linear, since the approximation of $\tilde{\mathcal{H}}_{\text{dis}}$ in \mathcal{H}_0 is itself a function of the $\{\sigma_{ab}\}$. This equation is thus self-consistent, and once the content of $\left\langle \tilde{\mathcal{H}}_{\text{dis}} \right\rangle_0$ will be made explicit, we will try the replica symmetric and the full RSB Ansatz as solutions of the saddle point equation (70), and hope that at least one of them will catch the main physics of the problem, without too many artifacts due to the variational method.

3.3.1 Detailed computation of the generic saddle point equation (69)

The variational procedure described in the section 3.2 begins by making explicit \mathcal{F}_0 and $\left\langle \tilde{\mathcal{H}}_{\text{el}} - \mathcal{H}_0 \right\rangle_0$, and taking their respective partial derivative $\partial_{G_{ab}(q)}$. Note that the limit $n \rightarrow 0$ is completely skipped thereafter, since we are approximating the $n \times n$ matrix of a replicated Hamiltonian, with n an arbitrary integer for the time being.

Since \mathcal{H}_0 is given by the parameters $\{G_{ab}^{-1}(q)\}$ and the Gaussian integrals pick up the inverse of the matrix describing the Hamiltonian, the thermal averages $\langle \mathcal{O} \rangle_0$ and the free energy \mathcal{F}_0 are functions of $\{G_{ab}(q)\}$. Since we have defined $\mathcal{F}_{\text{var}} \equiv F_0 + \left\langle \tilde{\mathcal{H}} - \mathcal{H}_0 \right\rangle_0$ and $\tilde{\mathcal{H}} \equiv \tilde{\mathcal{H}}_{\text{el}} + \tilde{\mathcal{H}}_{\text{dis}}$, the optimization condition (66) becomes here

$$\frac{\partial \mathcal{F}_{\text{var}}}{\partial G_{ab}(q)} \equiv \frac{\partial}{\partial G_{ab}(q)} \left(\mathcal{F}_0 + \left\langle \tilde{\mathcal{H}}_{\text{el}} - \mathcal{H}_0 \right\rangle_0 + \left\langle \tilde{\mathcal{H}}_{\text{dis}} \right\rangle_0 \right) = 0 \quad (71)$$

and gives a saddle point equation for the coefficients $\{G_{ab}^{-1}(q)\}$, which are again recovered through the Gaussian integrals of $\langle \cdot \rangle_0$.

We first compute $\mathcal{F}_0 = -\beta^{-1} \log Z_0$, using a discrete representation of the Fourier modes (cf. the section 1):

$$\begin{aligned} Z_0 &\equiv \int \mathcal{D}u_1(\dots) \mathcal{D}u_n \cdot e^{-\beta \mathcal{H}_0[\vec{u}]} \\ &= \int \mathcal{D}u_1(\dots) \mathcal{D}u_n \cdot e^{-\frac{\beta}{2} \int \frac{d^d \vec{q}}{(2\pi)^d} \sum_{ab} u_a^*(\vec{q}) G_{ab}^{-1}(\vec{q}) u_b(\vec{q})} \\ &= J \left(\prod_{q>0} \int \int du_1(q) du_1^*(q) (\dots) du_n(q) du_n^*(q) \right) \cdot e^{-\frac{\beta}{\Omega} \sum_{q>0} \sum_{ab} u_a^*(\vec{q}) G_{ab}^{-1}(\vec{q}) u_b(\vec{q})} \\ &= J \prod_{q>0} (\Omega \beta^{-1})^n \underbrace{\left(\prod_i \text{eigenvalues of } \hat{G}(q) \right)}_{\det \hat{G}(q)} = J \prod_{q>0} (\Omega \beta^{-1})^n \det \hat{G}(q) \end{aligned} \quad (72)$$

which implies that

$$\begin{aligned} \mathcal{F}_0 &= -\beta^{-1} \log Z_0 \\ &\stackrel{(72)}{=} -\beta^{-1} \sum_{q>0} \log \left(\det \hat{G}(q) \right) - \beta^{-1} \log \left(\underbrace{J \prod_{q>0} (\Omega \beta^{-1})^n}_{\text{cste}} \right) \end{aligned} \quad (73)$$

To make explicit $\partial\mathcal{F}_{\text{var}}/\partial G_{ab}(q)$, we need the matrix identity:

$$\frac{\partial}{\partial M_{ab}} \log(\det M) = (M^{-1})_{ab} \quad (74)$$

Thus

$$\frac{\partial\mathcal{F}_0}{\partial G_{ab}(q)} \stackrel{(73)}{=} -\beta^{-1} \sum_{\tilde{q}>0} \frac{\partial}{\partial G_{ab}(q)} \log(\det \widehat{G}(\tilde{q})) \stackrel{(74)}{=} -\beta^{-1} \cdot G_{ab}^{-1}(q) \quad (75)$$

As for $\langle \widetilde{\mathcal{H}}_{\text{el}} - \mathcal{H}_0 \rangle_0$, we have by definition:

$$\begin{aligned} \langle \widetilde{\mathcal{H}}_{\text{el}} - \mathcal{H}_0 \rangle_0 &= \left\langle \frac{1}{2} \int \frac{d^d q}{(2\pi)^d} \left(c(q) \sum_a u_a^*(q) u_a(q) - \sum_{ab} u_a^*(q) G_{ab}^{-1}(q) u_b(q) \right) \right\rangle_0 \\ &= \frac{1}{2} \int \frac{d^d q}{(2\pi)^d} \sum_{ab} (c(q) \delta_{ab} - G_{ab}^{-1}(q)) \langle u_a^*(q) u_b(q) \rangle_0 \\ &\stackrel{(24)}{=} \frac{1}{2} \int \frac{d^d q}{(2\pi)^d} \sum_{ab} (c(q) \delta_{ab} - G_{ab}^{-1}(q)) \cdot (2\pi)^d \beta^{-1} G_{ab}(q) \\ &= (2\pi)^d \beta^{-1} \cdot \frac{1}{2} \int \frac{d^d q}{(2\pi)^d} \left(c(q) \sum_{ab} \delta_{ab} G_{ab}(q) - \sum_{ab} G_{ab}^{-1}(q) G_{ab}(q) \right) \\ &= (2\pi)^d \beta^{-1} \cdot \frac{1}{2} \int \frac{d^d q}{(2\pi)^d} \left(c(q) \sum_a G_{aa}(q) - \sum_a 1 \right) \\ &= (2\pi)^d \beta^{-1} \cdot \frac{1}{2} \int \frac{d^d \tilde{q}}{(2\pi)^d} \cdot c(\tilde{q}) \cdot \sum_a G_{aa}(\tilde{q}) - \underbrace{(2\pi)^d \beta^{-1} \cdot \frac{1}{2}}_{\text{cste}} \end{aligned} \quad (76)$$

Since $c(q)$ and $G_{ab}(q)$ are symmetric for $\pm q$, it follows for its partial derivative:

$$\frac{\partial \langle \widetilde{\mathcal{H}}_{\text{el}} - \mathcal{H}_0 \rangle_0}{\partial G_{ab}(q)} = \beta^{-1} \cdot c(q) \cdot \delta_{ab} \quad (77)$$

Finally, combining the expressions (75) and (77), the optimization condition (71) becomes:

$$\begin{aligned} 0 &= \frac{\partial\mathcal{F}_{\text{var}}}{\partial G_{ab}(q)} = \frac{\partial}{\partial G_{ab}(q)} \left(\mathcal{F}_0 + \langle \widetilde{\mathcal{H}}_{\text{el}} - \mathcal{H}_0 \rangle_0 + \langle \widetilde{\mathcal{H}}_{\text{dis}} \rangle_0 \right) \\ &\stackrel{[\beta^{-1} \equiv T]}{=} -T G_{ab}^{-1}(q) + T c(q) \cdot \delta_{ab} + \frac{\partial}{\partial G_{ab}} \langle \widetilde{\mathcal{H}}_{\text{dis}} \rangle_0 \end{aligned}$$

which gives eventually the generic saddle point equation for the coefficients of the optimal \mathcal{H}_0 , at a finite temperature $T > 0$:

$$G_{ab}^{-1} = c(q) \cdot \delta_{ab} + \frac{1}{T} \frac{\partial}{\partial G_{ab}} \langle \widetilde{\mathcal{H}}_{\text{dis}} \rangle_0 \quad (78)$$

3.4 Saddle point equation for the variational Hamiltonian \mathcal{H}_0 of a 1D interface

To obtain the saddle point equation for the variational \mathcal{H}_0 applied to our model, we still have to make explicit in (70) the following thermal average:

$$\langle \widetilde{\mathcal{H}}_{\text{dis}} \rangle_0 = -\frac{1}{2} \beta D \int_{\mathbb{R}} \frac{d\lambda}{2\pi} \cdot e^{-\lambda^2 \xi^2} \int_{\mathcal{D}_z} dz \sum_{ab} \langle e^{i\lambda(u_a(z) - u_b(z))} \rangle_0 \quad (79)$$

before taking its partial derivative $\partial_{G_{ab}}$, and thus relate it to the coefficients $\{\sigma_{ab}\}$ defined by (70).

We have essentially to determine the thermal average of a generic λ mode (a Fourier mode *transversal* to the interface):

$$\langle e^{i\lambda(u_a(z) - u_b(z))} \rangle_0 = \exp \left[-\lambda^2 T \cdot \frac{1}{2} \int \frac{d^d q}{(2\pi)^d} (G_{aa}(q) + G_{bb}(q) - 2G_{ab}(q)) \right] \quad (80)$$

Actually $\langle e^{i\lambda(u_a(z)-u_b(z))} \rangle_0$ does not depend on z ; this shows again the translational invariance of the interface in the z direction, after averaging over disorder. In $\langle \tilde{\mathcal{H}}_{\text{dis}} \rangle_0$ the term $\int dz$ thus corresponds to the volume Ω of the system in the z direction, and physically the internal energy due to an ‘effective’ disorder Hamiltonian should indeed be extensive: $\langle \tilde{\mathcal{H}}_{\text{dis}} \rangle_0 \propto \Omega$. Using (80) in (79) in a discrete representation of the Fourier modes:

$$\langle \tilde{\mathcal{H}}_{\text{dis}} \rangle_0 = -\frac{1}{2}\beta D\Omega \int_{\mathbb{R}} \frac{d\lambda}{2\pi} e^{-\lambda^2 \xi^2} \sum_{a'b'} e^{-\lambda^2 T \cdot \frac{1}{\Omega} \sum_{\tilde{q}>0} (G_{a'a'}(\tilde{q}) + G_{b'b'}(\tilde{q}) - 2G_{a'b'}(\tilde{q}))} \quad (81)$$

Taking its partial derivative $\partial_{G_{ab}}$ and distinguishing the terms $a = b$ and $a \neq b$, we finally obtain for σ_{ab} , defined by (70):

$$\sigma_{a \neq b} = \frac{D}{T} \int_{\mathbb{R}} \frac{d\lambda}{2\pi} \cdot \lambda^2 \cdot e^{-\lambda^2 \xi^2} e^{-\lambda^2 T \int \frac{d^d \tilde{q}}{(2\pi)^d} (\tilde{G}(\tilde{q}) - G_{a \neq b}(\tilde{q}))} \quad (82)$$

$$\sigma_{aa} = -\sum_{a'} \sigma_{a' \neq a} \equiv \tilde{\sigma} \quad (83)$$

The variational method thus provides us with a self-consistent equation for the coefficients $\{G_{ab}^{-1}(q) = cq^2 - \sigma_{ab}\}$ of the optimal quadratic and replicated Hamiltonian \mathcal{H}_0 , to use in the computation of approximate thermal averages with replicas in our model. Indeed,

$$G_{a \neq b}^{-1}(q) = -\sigma_{a \neq b} \quad (84)$$

$$\tilde{G}^{-1}(q) = cq^2 - \tilde{\sigma} \quad (85)$$

$$G_c^{-1}(q) \equiv \sum_{a'} G_{aa'}^{-1}(q) = \tilde{G}^{-1}(q) - \sum_{a'} \sigma_{a' \neq a} = cq^2 \quad (86)$$

and the σ_{ab} coefficients are functions of the coefficients $\{G_{ab}\}$ which are accessible directly in the limit $n \rightarrow 0$ via the inversion formulas (45)-(49), given in the section 2.

As announced at the end of the section 3.3, the σ_{ab} do not depend on q . If there is no disorder, $D = 0$ and \mathcal{H}_0 is a diagonal matrix with coefficients cq^2 , as expected for a quadratic Hamiltonian of *uncoupled* elastic replicas. The irruption of disorder does not change the connected term $G_c^{-1} = cq^2$, it only populates the off-diagonal elements of \tilde{G}^{-1} with the q -independent terms $-\sigma_{a \neq b}$ and the diagonal one by what is needed to keep $G_c = \frac{1}{cq^2}$ invariant.

To move on to the computation of the roughness, we have now to find solutions of the equation (82), and hope that at least one of them will correspond to an approximative Hamiltonian \mathcal{H}_0 which will catch some of the physics of disorder. If we had worked directly with the exact effective replicated Hamiltonian $\tilde{\mathcal{H}}$, we would of course not have to choose between different solutions. In the next chapter, we will try two Ansätze and compute their corresponding roughness.

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