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Gibbs Thermodynamic Potentials for Disordered Systems

Maurizio Serva
Dipartimento di Matematica, Università dell'Aquila, I-67100 Coppito, L'Aquila, Italy

Giovanni Paladin
Dipartimento di Fisica, Università dell'Aquila, I-67100 Coppito, L'Aquila, Italy
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We propose a new method to estimate the quenched free energy in disordered systems. It uses generalized thermodynamic potentials, given by annealed averages of the partition function with appropriate constraints realized by the aid of Lagrange multipliers. The method is applied to Ising models with random magnetic fields. In that particular case, the constraints correspond to averaging only over the disorder configurations where the sum of the random variables has the correct mean value and variance.

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Disordered systems are characterized by two types of variables: the *hot* variables which arrange themselves to minimize the free energy and the *cold* variables which have much longer evolution times. A classical example is a spin glass with Hamiltonian $H_N=\sum_{i,j}J_{i,j}\sigma_i\sigma_j$ where the N spin variables $\sigma=\pm 1$ are of the first type and the random couplings J are of the second type. From the mathematical point of view this fact corresponds to two different kinds of averages. The typical free energy is thus given by the quenched average over the disorder *cold* variables

$$-(1/\beta N)\overline{\ln Z_N}=f_N\,, \tag{1}$$

where $Z_N=2^N\langle e^{-\beta H_N}\rangle_\sigma$ is given by a thermal average over the *hot* variables. In the thermodynamic limit, all the disorder realizations of $\{J_{i,j}\}$ (a part a set of zero probability measure) have the same free energy

$$\lim_{N\to\infty}-(1/\beta N)\ln Z_N(\{J_{i,j}\})=\lim_{N\to\infty}f_N=f\,. \tag{2}$$

This property is called self-averaging [1] since $(\ln Z_N)/N$ becomes a nonrandom quantity for $N\to\infty$. The calculation of the free energy in disordered systems is a difficult problem even in simple one-dimensional models. In practice, it is much easier to approximate the quenched average $\overline{\ln Z}$ by the annealed one $\ln(\overline{Z})$. From a physical point of view, this corresponds to allowing the *cold* variables to arrange themselves to minimize the free energy. As a consequence, the main contribution to the annealed free energy comes from a set of disorder realizations with zero probability measure in the limit $N\to\infty$. On a computational level, the annealed approximation gives a lower bound of f which is in most cases unsatisfactory.

The most celebrated method for the calculation of f is the replica trick [1], which permits one to find it by the continuation at $n=0$ of the annealed averages of the moments $\overline{Z^n}$ (for positive integer n), when there is no replica symmetry breaking.

This Letter proposes a quite different approach. We obtain an estimate of the quenched free energy in terms of annealed averages of Z where the relevant constraints are imposed by means of Lagrange multipliers. We thus get a generalized thermodynamic potential which is a function of the Lagrange multipliers, playing the role of the chemical potential in ordinary statistical mechanics. The advantage is that the set of disorder realizations which contributes to these potentials is much closer to the correct one. As a particular case, our method reproduces the very accurate results of the microcanonical method [2] for the Lyapunov exponent of product random matrices which are binomially distributed. However, it can be easily applied to continuous distributions and to problems which cannot be formulated in terms of transfer matrices as, e.g., mean-field theories.

Let us denote the free energy per spin at fixed coupling realization $\{J_{i,j}\}$ of an N spin system by

$$y = -(1/N\beta)\ln Z_N(\{J_{i,j}\}) . \quad (3)$$

In general, y is a random quantity which depends on the configuration $\{J_{i,j}\}$. In terms of the probability $P_N(y)dy$ that the free energy density falls in the interval $[y, y+dy]$, one thus has

$$\overline{\ln Z_N} = -\beta N \int dy\, P_N(y) y , \quad (4)$$

where the integral is over all possible values of y. For $N \to \infty$, the probability of finding $y \neq f$ should vanish, because of the self-averaging. Therefore for large N, $P_N(y)$ is peaked around the most probable value f, and one has

$$P_N(y) \sim e^{-S(y)N} , \quad (5)$$

where $S(y) > 0$ for $y \neq f$, and $S(f) = 0$, so that a saddle-point estimate of the integral gives the expected result [3]. In disordered systems, beyond y one can consider other intensive thermodynamic quantities defined in terms of the microscopic quenched variables. The simplest examples are $N^{-1}\sum_{i,j} J_{i,j}$ or $N^{-1}\sum_i h_i$ in Ising models with nearest-neighbor random couplings or with random magnetic fields.

Let us indicate by α one of these quantities, supposed to be self-averaging to $\bar{\alpha}$. In the previous cases, if $J_{i,j}$ and h_i are independent identically distributed random variables, α self-averages to $\bar{J}$ or to $\bar{h}$ because of the large number law. It follows that the joint probability $\mathcal{P}_N(y,\alpha) \sim \exp[-\mathcal{S}(y,\alpha)N]$ has a maximum at $y = f$, $\alpha = \bar{\alpha}$ which means that $\mathcal{S}(y,\alpha) > 0$ for $(y,\alpha) \neq (f,\bar{\alpha})$, and $\mathcal{S}(f,\bar{\alpha}) = 0$. Furthermore, since $P(y) = \int \mathcal{P}(y,\alpha) d\alpha$ one has from the saddle-point method

$$S(y) = \min_{\alpha} [\mathcal{S}(y,\alpha)] = \mathcal{S}(y,\alpha(y)) . \quad (6)$$

This equality obviously implies that $\alpha(f) = \bar{\alpha}$. The introduction of the new variable α has no effect in the integral $f = \int dy\, d\alpha\, \mathcal{P}(y,\alpha) y$ for the quenched free energy but is useful for later discussion because it shows that only the disorder realizations which correspond to $\alpha = \bar{\alpha}$ contribute to f in the thermodynamic limit.

The case of the annealed free energy

$$f_A \equiv \lim_{N \to \infty} -(1/N\beta)\ln(\bar{Z}_N) \quad (7)$$

is rather different. Taking into account only $P(y)$, one has

$$\bar{Z}_N = \int dy\, P_N(y) e^{-\beta y N} \sim \int dy\, e^{-N[S(y)+\beta y]} . \quad (8)$$

In the large-N limit this integral can be estimated by the saddle-point method so that

$$\beta f_A = \min_{y} [S(y) + \beta y] = S(y^*) + \beta y^* . \quad (9)$$

In general, y^* differs from the most probable value f and therefore $f_A \neq f$. On the other hand, we can consider the integral over the joint probability measure $\mathcal{P}(y,\alpha)dy\,d\alpha$, so that one has

$$\beta f_A = \min_{y,\alpha} [\mathcal{S}(y,\alpha) + \beta y] = \mathcal{S}(y^*,\alpha^*) + \beta y^* , \quad (10)$$

where $\alpha^* = \alpha(y^*)$. The above expression is the same as (9) but explicitly shows that the minimum condition is realized for a free energy $y = y^*$ and for $\alpha = \alpha^*$. These two quantities both differ from the quenched averages f and $\bar{\alpha}$. In other words, the main contributions to f_A come from disorder realizations which are different from those contributing to f. At this point, it would be clearly useful to minimize expression (10) imposing $\alpha = \bar{\alpha}$. This is indeed possible by means of a Lagrange multiplier μ. In the following we take $\bar{\alpha} = 0$, to simplify the notation. In order to average over the disorder configurations with $\alpha = \bar{\alpha} = 0$, we start by computing

$$\overline{Ze^{-\mu\alpha N}} = \int \mathcal{P}(y,\alpha) e^{-\beta y N} e^{-\mu\alpha N} \sim e^{-g(\beta,\mu)N} , \quad (11)$$

where we have introduced the new thermodynamic potential

$$g(\beta,\mu) = \min_{y,\alpha} [\mathcal{S}(y,\alpha) + \beta y + \mu\alpha] . \quad (12)$$

The value $\tilde{\mu}$ of the Lagrange multiplier which fixes $\alpha = \bar{\alpha} = 0$ is given by the condition

$$\left. \frac{d \ln \overline{Ze^{-\mu\alpha N}}}{d\mu} \right|_{\tilde{\mu}} = -\left. \frac{dg(\beta,\mu)}{d\mu} \right|_{\tilde{\mu}} = 0 . \quad (13)$$

At fixed β, the variable α can therefore be expressed as a function of the Lagrange multiplier, i.e., $\alpha(\mu) = dg/d\mu$. The two relations (12) and (13) give $g(\beta,\tilde{\mu})$ (the maximum of a Gibbs-like potential) as the Legendre transform of the annealed free energy f_A (a Helmholtz-like potential). As the minimum of α in (12) for $\mu = \tilde{\mu}$ is reached at $\alpha = 0$, one has

$$g(\beta,\tilde{\mu}) = \min_{y} [\mathcal{S}(y,0) + \beta y] = \mathcal{S}(\tilde{y},0) + \beta\tilde{y} , \quad (14)$$

which should be compared with (10), where $\alpha = \alpha^*$ is a free parameter different from its self-average $\bar{\alpha} = 0$. Furthermore, by the convexity of the logarithm function, one can prove the inequality

$$f \geq g(\beta,\tilde{\mu}) \geq f_A \equiv g(\beta,\mu = 0) , \quad (15)$$

showing that the Gibbs potential is a better approximation of f than the annealed free energy. In fact, $g(\beta,\tilde{\mu}) - f_A$ has an important physical meaning. When αN is considered as the sum of hot variables, the system minimizes the annealed free energy $f_A = g(\beta,0)$, while when α is correctly taken as a cold variable, the system cannot arrange itself and it should minimize $g(\beta,\tilde{\mu})$. In other words, $W \equiv g(\beta,\tilde{\mu}) - f_A = \int_0^{\tilde{\mu}} \alpha(\mu) d\mu$ is the work needed to freeze the variable α. This consideration indicates that a macroscopic variable can be of two types: (1) $W = 0$. In the thermodynamic limit the variable is not relevant since no work is needed to freeze it. It follows that $\tilde{\mu} = 0$ and $g = f_A$. (2) $W > 0$. One obtains a better approximation of the quenched free energy f by comput-

ing $g(\beta,\tilde{\mu})$ instead of f_A, since $\tilde{\mu}\neq 0$ and $g(\beta,\tilde{\mu})$ is strictly larger than f_A.

Our arguments can be trivially extended to a set of M relevant variables $\{\alpha_i\}$. Such a set will be complete only if $g(\beta,\tilde{\mu}_1,\ldots,\tilde{\mu}_M)=f$ and it might be rather difficult to individuate it. For instance, it would be very interesting to understand what are the relevant variables in the Sherrington-Kirkpatrick model where there is a replica symmetry breaking in the spin-glass phase.

To illustrate our method, in the following we study two models where the introduction of few relevant variables allows us to recover the exact solution, or to get an extremely good approximation of f.

Let us start with an infinite-range random-field Ising model with Hamiltonian

$$H=\sum_{i>j}J\sigma_i\sigma_j+\sum_i h_i\sigma_i\,, \tag{16}$$

where J is a constant coupling and the magnetic fields h_i are independent identically distributed random variables with zero mean value. In this model $\ln\overline{Z}\neq\overline{\ln Z}$, indicating the presence of at least one relevant variable besides y. Let us limit ourselves to considering the disorder realizations of $\{h_i\}$ that satisfy the law of the large numbers, that is,

$$a=\frac{1}{N}\sum_i^N h_i=0\,. \tag{17}$$

We can thus compute the annealed average over the h distribution,

$$\overline{Ze^{-\mu aN}}=\sum_{\{\sigma_i=\pm 1\}}\exp\left[\frac{1}{N}\sum_{i>j}J\sigma_i\sigma_j+\sum_i h_i(\sigma_i+\mu)\right],$$

where $\beta=1$ is chosen for simplicity. Using the independence of the random variables h_i, the average over the disorder can be performed:

$$\sum_{\{\sigma_i=\pm 1\}}\exp\left[\frac{1}{N}\sum_{i>j}J\sigma_i\sigma_j\right]\overline{\exp\left[\sum_i h_i(\sigma_i+\mu)\right]}\,. \tag{18}$$

To be explicit, we consider the binomial distribution $h_i=\pm h$ with respective weights $\frac{1}{2}$, so that (18) takes the form

$$\sum_{\{\sigma_i=\pm 1\}}\exp\left[\frac{1}{N}\sum_{i>j}J\sigma_i\sigma_j\right]\prod_i^N\cosh\left[h(\sigma_i+\mu)\right]. \tag{19}$$

One should note the identity

$$\cosh[h(\sigma_i+\mu)]=\exp[A(\mu)+B(\mu)\sigma_i]\,,$$

where A and B are solutions of the equations

$$\cosh[h(1+\mu)]=\exp[A(\mu)+B(\mu)]$$

and

$$\cosh[h(-1+\mu)]=\exp[A(\mu)-B(\mu)]\,,$$

obtained by taking $\sigma_i=\pm 1$. After some trivial algebraic manipulations, one thus gets

$$\overline{Ze^{-\mu aN}}=\sum_{\{\sigma_i=\pm 1\}}\exp\{N[A(\mu)+\tfrac{1}{2}Jm^2+B(\mu)m]\}\,, \tag{20}$$

where $m\equiv\sum_i\sigma_i/N$ is the magnetization density. The sum over the thermal configurations can be transformed into an integral over the magnetization, that is,

$$\int P(m)dm\exp\{N[A(\mu)+\tfrac{1}{2}Jm^2+B(\mu)m]\}\,, \tag{21}$$

where $P(m)$ is given by the binomial factor and can be approximated for large N by the Stirling formula as $P(m)\sim\exp[-s(m)N]$ with

$$s(m)=\frac{(1-m)}{2}\ln\frac{(1-m)}{2}+\frac{(1+m)}{2}\ln\frac{(1+m)}{2}\,. \tag{22}$$

The usual saddle-point estimation of (21) gives

$$g(\beta=1,\mu)=A(\mu)+\tfrac{1}{2}J(m^*)^2+B(\mu)m^*-s(m^*)\,, \tag{23}$$

where m^* is the value of m maximizing the exponent in the integral. The exact solution for f (see Ref. [4]) coincides with $g(\beta,\tilde{\mu})$ where $dg/d\mu|_{\tilde{\mu}}=0$. Our result shows that $\sum_i h_i$ is the only new relevant thermodynamic variable in this mean-field model.

Let us now describe a less trivial model where one constraint is not sufficient to get the quenched free energy by the Gibbs potential. It is the one-dimensional Ising model with Hamiltonian

$$H=\sum_i J\sigma_i\sigma_{i+1}+\sum_i h_i\sigma_i\,,$$

where J is a positive coupling and $h_i=a+b\omega_i$ is a random field with a,b arbitrary constants and ω_i independent random variables identically distributed according to a standard Gaussian. One can repeat the previous calculation for the Gibbs potential introducing the variable $a=\sum\omega_i/N$ to obtain

$$e^{-g(\beta=1,\mu)N}=\sum_{\{\sigma_i=\pm 1\}}\prod_i^N\exp[J\sigma_i\sigma_{i+1}+a\sigma_i]\overline{\exp[\omega_i(b\sigma_i+\mu)]}=e^{(b^2+\mu^2)N/2}\sum_{\{\sigma_i=\pm 1\}}\prod_i^N\exp[J\sigma_i\sigma_{i+1}+(a+b\mu)\sigma_i]\,,$$

where the disorder average is performed by an integral over the standard Gaussian $P(\omega)=(2\pi)^{-1/2}\exp(-\omega^2/2)$. The resulting thermodynamic potential is given by the solution of a one-dimensional Ising model under constant magnetic field $H=a+b\mu$. The free energy of such a model is well known to be

$$\gamma(H)=e^J\cosh(H)+[e^{2J}\cosh^2(H)-2\sinh(2J)]^{1/2}\,, \tag{24}$$

so that the Gibbs thermodynamic potential is

$$g(\beta=1,\mu)=-\tfrac{1}{2}(b^2+\mu^2)-\ln\gamma(H[\mu])\,. \tag{25}$$

Although $g(\beta,\tilde{\mu})$ is a much better approximation of the quenched free energy than the annealed free energy $g(\beta,\mu=0)$, it is still different from f, as shown in Fig. 1. In fact, we can impose a further natural constraint on the system by considering only the disorder realizations that have the correct mean value and variance for the total magnetic field, i.e., the realizations where, besides $a=0$, one also has $a_2=\sum_i^N(\omega_i^2-1)/N=0$. To do it, we introduce a second Lagrange multiplier μ_2 related to the new variable a_2, as well as the generalized thermodynamic potential $g_2(\beta,\mu,\mu_2)$ defined by the relation

$$e^{-g_2(\beta=1,\mu,\mu_2)N}=\sum_{\{\sigma_i=\pm 1\}}\prod_i^N \exp[J\sigma_i\sigma_{i+1}+a\sigma_i]\overline{\exp[\omega_i(b\sigma_i+\mu)+\mu_2(\omega_i^2-1)]}\,.$$

After some trivial Gaussian integrations, the problem is again reduced to the solution of an appropriate one-dimensional Ising model without disorder which has free energy given by (24). One thus finds

$$g_2(\beta=1,\mu,\mu_2)=-\mu_2-\frac{b^2+\mu^2}{2(1-2\mu_2)}-\tfrac{1}{2}\ln(1-2\mu_2)-\ln\gamma(H[\mu,\mu_2])\,, \quad (26)$$

with $H=a+b\mu/(1-2\mu_2)$. The potential g_2 becomes equal to g for $\mu_2=0$. The maxima of g_2 are reached at $\mu=\tilde{\mu}_1$, $\mu_2=\tilde{\mu}_2$ given by the relations

$$\left.\frac{\partial g_2}{\partial\mu}\right|_{\tilde{\mu}_1,\tilde{\mu}_2}=\left.\frac{\partial g_2}{\partial\mu_2}\right|_{\tilde{\mu}_1,\tilde{\mu}_2}=0\,.$$

Figure 1 shows the potentials $-g$ and $-g_2$ whose minima give increasingly better estimates of the quenched free energy. The exact solution of the model is not known. However, two constraints are not sufficient to obtain f by the corresponding generalized potential. It is an open issue whether the number of intensive variables $\{\alpha_i\}$ needed here is finite or not.

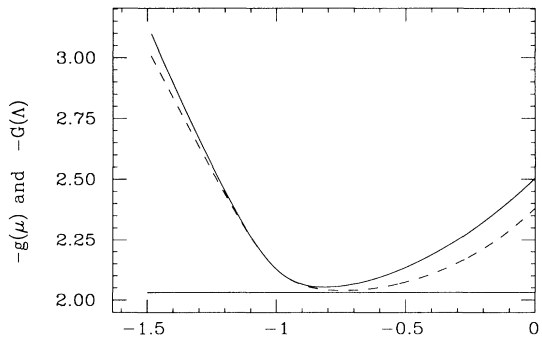

FIG. 1. Ising model with $J=1$ and random magnetic field $h_i=a+b\omega_i$ ($a=1$, $b=1$, and ω_i normal Gaussian variables). The solid line is the Gibbs potential $-g(\beta=1,\mu)$ and the dashed line is $-G(\Lambda)=\min_\mu-\tilde{g}_2(\beta=1,\mu,\Lambda)$ with $\tilde{g}_2(\beta=1,\mu,\Lambda(\mu,\mu_2))=g_2(\beta=1,\mu,\mu_2)$ and $\Lambda=\mu/(1-2\mu_2)$. The straight line indicates the numerical result for the quenched free energy $f=2.031\pm0.001$. Our approximations are obtained by taking the minima of the thermodynamic potentials, that is, $-g(\beta=1,\tilde{\mu}=-0.81)=2.0530$ and $-G(\tilde{\Lambda}=-0.75)=2.0389$ (corresponding to the values $\tilde{\mu}_1=-0.489$, $\tilde{\mu}_2=0.198$). The annealed free energy is obtained by $-g(\beta=1,\mu=0)=2.5029$.

Finally, we want to mention that our method can be applied to estimate the maximum Lyapunov exponent of products of random matrices which describe many interesting physical phenomena [5] such as the localization of electrons in random potential (Anderson model).

Our methods could also be useful to get a deeper understanding of highly frustrated systems. In these cases, nontrivial combinations of the random couplings (or fields) should be necessary to define a *relevant* variable α. For instance, the variable $\alpha=N^{-1}\sum J_{i,j}$ is frozen without work in the Sherrington-Kirkpatrick model, while we expect that good results can be obtained by fixing the number of frustrated triples.

In conclusion, we have found a general tool for the calculation of quenched averages, extending the notion of thermodynamic potentials to disordered systems. Its range of applicability is extremely wide, varying from infinite-range models to products of transfer random matrices. It can compete with the replica trick for practical purposes, and it also allows one to individualize the macroscopic variables which control the disorder. The major problem is its application to spin glasses with replica symmetry breaking where the challenge is the determination of the relevant variables.

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