Random matrix theory and the statistical mechanics of disordered systems

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Abstract. A new method, that systematically combines results of random matrix theory and the usual statistical mechanics, is described to study thermodynamic properties of disordered systems. Two exactly solvable models are examined in this formulation to illustrate the usefulness of this method for systems described by random as well as non-random Hamiltonian.

Keywords. Random matrices; statistical mechanics; disordered systems; thermodynamic properties

1. Introduction

This paper describes a general statistical approach, to obtain thermal properties of a system for which only partial information is available concerning its initial state as well as its Hamiltonian. Clearly, such an approach would be useful in the study of various kinds of disordered systems (Ziman 1979; Balian *et al* 1978). Since a certain amount of ignorance regarding both the initial state and the Hamiltonian is acknowledged the aim here is to combine the basic ideas of statistical mechanics (Khinchin 1949) and random matrix theory(RMT) (Porter 1965; Mehta 1967) for developing a theory of disordered systems. It should be stressed that although a great deal of work has been done on disordered systems, and that there have been studies (Kosterlitz *et al* 1976) which have used some results of RMT, there has been no systematic attempt to unify the two statistical theories to formulate a theory for disordered systems.

The basic point is that, during the last two decades, a great deal has been learnt (Porter 1965; Mehta 1967; Brody *et al* 1981) about the average and the fluctuation properties of energy (eigenvalue) spectra, resulting from different types of Hamiltonian ensembles. For example, one knows the asymptotic form of the ensemble-averaged level density (inverse Laplace transform of the partition function), the two-point correlation function (which is related to specific fluctuation measures) and so on. It seems worthwhile therefore to find out the way in which these spectral quantities contribute to the thermal properties of disordered systems. Clearly it is also very important to find out whether such an approach leads to simplicities, new insights and results.

In view of these considerations, Hamiltonian ensembles are introduced in §2 in a general way and the statistical mechanics of systems described by such (Hamiltonian) ensembles is developed. It is shown that the average and the fluctuation properties

of the energy levels (of the Hamiltonian ensemble) appear in a very natural way in the description of the thermodynamics of the system.

The general statistical framework developed in §2 is then applied to two extremely simple systems. In §3 a finite system of non-interacting particles having random energies is studied. Section 4 contains the determination of the thermal properties of the infinite range Ising model of Kac (Kac 1968; Stanley 1971). Although the Hamiltonian of the Kac model is not random it turns out that cumulant expansions (Cramer 1946) can be profitably used. The purpose of studying these two exactly solvable models is to demonstrate the use of the new method for random and non-random systems. Finally § 5 contains a summary and some concluding remarks.

2. Statistical mechanics of Hamiltonian ensembles

As usual (Ziman 1979; Balian *et al* 1978) the first step towards describing a disordered system is to define an ensemble of Hamiltonians, which incorporates what is known about the Hamiltonian and randomizes what is not known. Following the RMT (Porter 1965; Mehta 1967) approach, the unknown features are described by means of random variables, having specified distributions over the ensemble.

Consider a system of n particles (distinguishable or indistinguishable), which interact *via* a random k-body interaction. For convenience of representation, each of the n particles is supposed to be in one of the Ω possible single particle states that are all degenerate in energy. The only (physical) restrictions on n, k and Ω are $k \leqslant n$ and for fermions $n \leqslant \Omega$. The Hamiltonian ensemble of the system is then defined by (1) and (2) which follow:

$$H(k) = \sum_{\alpha \leqslant \beta} W_{\alpha\beta}(k) \, A_{\alpha}^{+}(k) \, A_{\beta}(k).$$

(1)

Here $A_{\alpha}^{+}(k)$ and $A_{\beta}(k)$ are respectively the creation and destruction operators for k particles in the states α and β. The states α, β have the permutation symmetry appropriate to the nature of particles. The sum in (1) goes over all distinct k-particle states and their total number is denoted by $d(k)$. $W_{\alpha\beta}(k) = \langle k \, \alpha \, | H | \, k \, \beta \rangle$ is the matrix element of H between the states α and β, and it is assumed to be real and symmetric *i.e.* $W_{\alpha\beta}(k) = W_{\beta\alpha}(k)$. The $W_{\alpha\beta}$'s are taken to be independent random variables having a distribution $p(W_{\alpha\beta})$. If $p(W_{\alpha\beta})$ is a Gaussian with mean zero and variance v^2 over the ensemble then

$$p(W_{\alpha\beta}) = \frac{1}{(2\pi v^2)^{1/2}} \exp(-W_{\alpha\beta}^2 / 2\, v^2).$$

(2)

Thus the Hamiltonian ensemble in the k-particle space is defined by a set of $d(k) \times d(k)$ symmetric square matrices. The different matrix elements are independent having (say) the distribution in (2). Actually the system contains n particles, and hence, the matrix elements of $H(k)$ between all distinct n-particle states need to be evaluated for the determination of the physical properties of the system. One therefore has for the n-particle system, an ensemble of $d(n) \times d(n)$ Hamiltonian matrices, but

the matrix elements are not all independent. The average and fluctuation properties of the eigenvalue distributions of such random Hamiltonians have been studied (French and Wong 1970; Bohigas and Flores 1971; Mon and French 1975) in the last few years, and have been reviewed recently (Brody *et al* 1981).

It should be pointed out that the system described by such an (Hamiltonian) ensemble has a bounded energy spectrum, and it may therefore seem that this would restrict the applicability of the method to 'finite' systems only. However, it is known from the use of these methods to the nuclear level density problem (French and Chang 1972), that by partitioning the configuration space into sub-spaces, calculating the number of levels (finite) in each subspace and then adding them over all the sub-spaces, it is possible to overcome this difficulty and obtain results that are reliable to any specified excitation energy. It seems likely that the same procedure (of partitioning) would in the present context also allow one to deal with systems that do not have a bounded energy spectrum.

In order to theoretically obtain thermal properties of such a disordered system, it is necessary to work out the statistical mechanics for the ensemble of H defined by (1) and (2). It is obvious that this implies carrying out averages of the appropriate physical quantities over the Hamiltonian ensemble and the usual statistical (Gibbs) ensemble. Thus, one must know the partition function $\langle Z(\beta) \rangle$ or the free energy $\langle F(\beta) \rangle$ of the system, as a function of the parameter $\beta = 1/kT$ where k is the Boltzmann constant and T the absolute temperature. The brackets in the quantities $\langle Z(\beta) \rangle$, $\langle F(\beta) \rangle$ denote averages over the Hamiltonian ensemble. More precisely, if the statistical ensemble is canonical, one has

$$\langle Z(\beta) \rangle = \int dE \, \langle \rho(E) \rangle \exp(-\beta E), \tag{3}$$

$$\beta \langle F(\beta) \rangle = - \langle \ln Z(\beta) \rangle. \tag{4}$$

In (3) $\langle \rho(E) \rangle$ denotes the level density averaged over the Hamiltonian ensemble. Also it should be noted that in general $\langle \ln Z(\beta) \rangle \neq \ln \langle Z(\beta) \rangle$. As is well known (Ziman 1979; Balian *et al* 1978) for 'annealed' systems one must determine $\ln \langle Z(\beta) \rangle$ and for 'quenched' systems $\langle \ln Z(\beta) \rangle$. Let us first consider $\langle Z(\beta) \rangle$. Clearly in order to evaluate $\langle Z(\beta) \rangle$, one needs the form of the ensemble-averaged level density $\langle \rho(E) \rangle$.

As regards the form of the ensemble-aveaged eigenvalue distribution, there are by now some well-established asymptotic results (French and Wong 1970; Bohigas and Flores 1971; Mon and French 1975). These are

(a) If $n \to \infty$ and $\Omega \to \infty$ such that $n/\Omega \to 0$ and if all the particles interact simultaneously ($k = n$) then $\langle \rho(E) \rangle$ is a semicircle.

(b) Under the same conditions for n and Ω but with $k \ll n$, $\langle \rho(E) \rangle$ is a Gaussian.

(c) For intermediate cases, ($k \neq n$, k not very much greater than n) $\langle \rho(E) \rangle$ takes a characteristic form that can be defined in terms of its moments.

Although the results in (b) and (c) have been proved for fermions, they also hold for bosons and for distinguishable particles. It should also be pointed out that the Gaussian form in (b) results as a consequence of the central limit theorem (CLT) and some of its generalizations.

For many physical situations, the conditions described in (b) seem to be fulfilled—*i.e.* the system has a very large number of particles, it is dilute ($n/\Omega \to 0$) and the interactions are always of low particle rank, like one-body and two-body. Thus in all such cases one knows $\langle \rho(E) \rangle$ and it should, in principle, be possible to determine $\langle Z(\beta) \rangle$ (ln $\langle Z(\beta) \rangle$) and obtain the thermal properties of the system. It should be pointed out that only the (global) average property of the eigenvalue distribution ($\langle \rho(E) \rangle$) determines the thermal properties of an 'annealed' system. The local fluctuation properties of the ensemble are of no consequence for this purpose.

Let us now consider a 'quenched' system. For this purpose one expands for each Hamiltonian in the ensemble the level density $\rho(E)$ and the partition function $Z(\beta)$ about their respective ensemble averages

$$\langle \rho(E) \rangle \text{ and } \langle Z(\beta) \rangle,$$

i.e.

$$\rho(E) = \langle \rho(E) \rangle + \delta\rho(E) \tag{5}$$

$$Z(\beta) = \langle Z(\beta) \rangle + \delta Z(\beta), \tag{6}$$

where $\langle Z(\beta) \rangle$ is defined in (3),

and $$\delta Z(\beta) = \int dE \, \delta\rho(E) \exp(-\beta E). \tag{7}$$

Note that $\langle \delta Z(\beta) \rangle = 0$ since by definition $\langle \delta\rho(E) \rangle = 0$. Taking the ensemble average of ln $Z(\beta)$ one gets

$$\langle \ln Z(\beta) \rangle = \langle \ln [\langle Z(\beta) \rangle + \delta Z(\beta)] \rangle,$$

$$= \ln \langle Z(\beta) \rangle + \left\langle \ln \left(1 + \frac{\delta Z(\beta)}{\langle Z(\beta) \rangle}\right) \right\rangle. \tag{8}$$

In the second term on the right side the function

$$\ln \left(1 + \frac{\delta Z(\beta)}{\langle Z(\beta) \rangle}\right)$$

can be expanded in a series provided $|\delta Z(\beta)/\langle Z(\beta) \rangle| < 1$. Clearly, this requires that for each Hamiltonian in the ensemble, the contribution to the partition function coming from $\delta\rho(E)$ (equation (5)) should be quite small compared to that from the ensemble-averaged level density $\langle \rho(E) \rangle$. Assuming this to be the case one obtains (with $\langle \delta Z(\beta) \rangle = 0$).

$$\langle \ln Z(\beta) \rangle = \ln \langle Z(\beta) \rangle - \frac{1}{2} \frac{\langle [\delta Z(\beta)]^2 \rangle}{\langle Z(\beta) \rangle^2} + \frac{1}{3} \frac{\langle [\delta Z(\beta)]^3 \rangle}{\langle Z(\beta) \rangle^3} + \cdots \tag{9}$$

It is easy to show that $\langle [\delta Z(\beta)]^2 \rangle$ is given by

$$\langle [\delta Z(\beta)]^2 \rangle = \int dE_1 \int dE_2 \, \langle \delta\rho(E_1) \, \delta\rho(E_2) \rangle \exp[-\beta(E_1 + E_2)], \tag{10}$$

where $\qquad \langle \delta \rho (E_1) \, \delta \rho (E_2) \rangle = \langle \rho (E_1) \, \rho (E_2) \rangle - \langle \rho (E_1) \rangle \langle \rho (E_2) \rangle \equiv S^\rho (E_1, E_2).$ (11)

$S^\rho (E_1, E_2)$ is the two-point function (Brody *et al* 1981). The higher order terms $\langle [\delta Z (\beta)]^k \rangle$ are similarly related to the k-point function $S^\rho (E_1, E_2, ... E_k)$. These k-point functions for the three-standard ensembles (Mehta 1967) have been evaluated by Dyson (Dyson 1970; Mehta 1971). Thus, at least in principle one can evaluate the various terms in (9). If it turns out (as in the case of nuclear spectra (Brody *et al* 1981)), that the most interesting fluctuation measures depend only on the density $\langle \rho (E) \rangle$ and the two-point function $S^\rho (E_1, E_2)$, then the task is much simpler.

It is clear from this development that the fluctuation properties of the energy spectra are essential in the description of the thermal properties of quenched systems. This was not the case for annealed systems.

As mentioned earlier, two very simple systems are studied next to illustrate some of these ideas.

3. Non-interacting particles with random energies

Consider a system of n distinguishable non-interacting particles distributed in Ω single particle states, and let ϵ_i $(i = 1...n)$ be the energy (random) of the ith particle. ϵ_i's are then random variables, which are assumed to be distributed identically and independently according to some probability function $p(\epsilon_i)$, with (say) mean $\bar{e}$ and variance v^2. The total energy $E = \Sigma \epsilon_i$ is also a random variable, having (due to CLT) a Gaussian distribution asymptotically $(n \to \infty)$. If $\langle \rho(E) \rangle$ is not exactly a Gaussian but close to it then one can expand it about a Gaussian. The complete expansion (Cramer 1946) in terms of the variable $x = (E - \bar{E})/\sigma$, where $\bar{E}$ and σ^2 are respectively the centroid and the variance of the distribution, is

$$\langle \rho (x) \rangle = \frac{d(n)}{\sqrt{2\pi}} \exp (-x^2/2) \left[1 + \sum_{p=3}^{\infty} (h_p/p!) H_p (x) \right].$$ (12)

Here H_p is Hermite polynomial of order p and the coefficients h_p can be expressed in terms of the normalized cumulants K_p. Writing the lowest few terms explicitly one has

$$\langle \rho (x) \rangle = \frac{d(n)}{\sqrt{2\pi}} \exp (-x^2/2) \left[1 + \frac{K_3}{3!} (x^3 - 3x) + \frac{K_4}{4!} (x^4 - 6x^2 + 3) + ... \right]$$

Note that in the present case $\bar{E} = n\bar{e}$, $\sigma^2 = nv^2$, $d(n) = \Omega^n$, and K_3 and K_4 are respectively the skewness and the excess parameters for the n particle distribution. It should be noted that $K_3 \sim (n)^{-1/2}$ and $K_4 \sim (n)^{-1}$.

A number of general remarks need to be made about the series expansion (equation (12)) of the density in terms of the moments (cumulants). From formal considerations alone, such an expansion is meaningful if the series converges and also if the density is uniquely determined by its moments. The question of real interest to us however is to examine whether a severely truncated series involving only the lowest few

cumulants, can provide a satisfactory approximation to the level density, so far as the thermal properties are concerned. It must be stressed that using only a few terms in the series may cause serious problems such as (i) the density function may become negative for some values of the argument near the tails of the distribution and (ii) inclusion of more terms in the expansion may not lead to an improvement in the approximation to the density. Although these disadvantages exist, the great usefulness of the expansion (if used with caution) is in providing a direct link between spectral properties and thermal properties of a system.

If one retains only the first term in the expansion of $\langle \rho(x) \rangle$ while evaluating $\langle Z(\beta) \rangle$ (equation (3)), one obtains

$$\langle Z(\beta) \rangle = d(n) \exp\left(\frac{nv^2 \beta^2}{2} - n\bar{e}\,\beta\right).$$

Furthermore, it is obvious and also easy to show in this case that the free energy,

$$\langle F(\beta) \rangle \equiv -\frac{1}{\beta} \langle \ln Z(\beta) \rangle = -\frac{1}{\beta} \ln \langle Z(\beta) \rangle,$$

and hence finds for $\langle F(\beta) \rangle$

$$\langle F(\beta) \rangle = -\frac{1}{\beta} \ln d(n) - \frac{1}{\beta}\left(\frac{nv^2 \beta^2}{2} - n\bar{e}\,\beta\right).$$

From $\langle F(\beta) \rangle$ one obtains the various thermodynamic properties.

Pressure: $P = -\partial \langle F \rangle / \partial \Omega = nkT/\Omega.$ (13)

Equation of state: $P\Omega = nkT.$ (14)

Internal energy: $U = \langle F \rangle - kT\left(\frac{\partial \langle F \rangle}{\partial (kT)}\right) = -\frac{nv^2}{kT} + n\bar{e}.$ (15)

Specific Heat at constant Ω: $C_\Omega = (\partial U/\partial T)_\Omega = nv^2/kT^2.$ (16)

Enthalpy: $H = U + P\,\Omega = -\frac{nv^2}{kT} + n\bar{e} + nkT.$ (17)

Specific Heat at constant P: $C_P = \frac{nv^2}{kT^2} + nk.$ (18)

$$C_P - C_\Omega = nk. \tag{19}$$

Note that the number of single particle states Ω can be directly related to the volume, and hence (13), (14) and (19) correspond exactly to the results for a perfect monoatomic gas. The difference in results (equations (15)–(18)) between the system considered here and the perfect gas arises from the fact that, in contrast to the latter

system the former does not allow the energy ϵ of a single particle to be infinite. It is also worthwhile to point out that the $1/T^2$ dependence of C_Ω is a consequence of the cumulants K_p ($p > 2$) being zero for a Gaussian level density $\langle \rho(E) \rangle$. The higher cumulants would give a contribution proportional to T^{-p} ($p > 2$) to C_Ω.

It is clear (from this example) that a system having a Gaussian energy level density will not display any critical behaviour with temperature. The importance and outcome of including terms proportional to $(n)^{-1/2}$, $(n)^{-1}$ etc. in the expansion of $\langle \rho(x) \rangle$ (equation (12)) will be discussed separately.

4. Ising interaction with infinite range

Following Kac (1968), let us consider a model in which each spin interacts equally with all the other spins in the lattice. The Hamiltonian for a system of n spins is (Stanley 1971)

$$H = -\frac{2J}{n} \sum_{i<j} s_i \, s_j, \tag{20}$$

where each $s_i = \pm 1$ ($i = 1, 2 \dots n$) and the strength $J > 0$. The partition function Z_n is

$$Z_n = \sum_{s_1} \sum_{s_2} \dots \sum_{s_n} \exp(-\beta H). \tag{21}$$

In order to evaluate Z_n let us introduce a new 'collective' variable S, where

$$S = \sum_{i=1}^{n} s_i.$$

In terms of S one can write Z_n (by changing summation over the s_i's to an integral over S), as

$$Z_n = \int_{-n}^{n} dS \, \rho(S) \exp[-\beta(J - JS^2/n)], \tag{22}$$

where $\rho(S)$ is the density of states for the n spins. As before, by applying CLT to the random variable S, one gets asymptotically a Gaussian form for $\rho(S)$. For finite n one has the expansion given in (12). If only the asymptotic (Gaussian) term is included in evaluating Z_n, one has (with $\bar{S} = 0$ and $\sigma^2(S) = \overline{S^2} - (\bar{S})^2 = n$)

$$Z_n = \frac{d(n) \exp(-\beta J)}{(2\pi\sigma^2)^{1/2}} \int_{-n}^{n} ds \exp(Cs^2/n),$$

where $C = \beta J^{-1/2}$. There are two distinct cases now depending upon whether $C < 0$ or $C > 0$. In both the cases the integral Z_n can be evaluated exactly. Knowing Z_n, we evaluate $\bar{g}$, the free energy per spin, in the thermodynamic limit, which is defined as,

$$\bar{g} = - kT \lim_{n \to \infty} \left[\frac{1}{n} \ln Z_n \right]. \tag{23}$$

It turns out that in the two cases

$$\bar{g} = - kT \ln 2, \quad (C < 0), \tag{24}$$

and

$$g = - kT \ln 2 - kT \left(\frac{J}{kT} - \frac{1}{2} \right). \tag{25}$$

$\bar{g}$ thus has an additional contribution below a 'critical' temperature $kT_c = 2J(C = 0)$. It can also be verified that the spontaneous magnetization is zero for $T \gtrless T_c$ and indeterminate for $T = T_c$. Furthermore, the specific heat C_v is zero for all T. It is clear therefore that the approximation used is unable to reproduce the results of mean field theory or the Kac model (Kac 1968; Stanley 1971). The problem is that one has introduced the asymptotic form $(n \to \infty)$ for $\rho(S)$ in the partition function, before taking the thermodynamic limit. To be consistent one ought to retain higher order terms in $(n)^{-1}$ in $\rho(x)$ (equation (12)) while evaluating Z_n, and then take the thermodynamic limit. It should be pointed out that the 'collective' variable S represents physically the spontaneous magnetization of the system and as mentioned earlier has asymptotically a Gaussian distribution with mean zero ($\bar{S} = 0$) and variance n. Therefore, for values of S close to the centroid $\bar{S} = 0$, one is justified in retaining in the expansion of $\rho(S)$ (about the asymptotic Gaussian form) terms involving only the lowest few cumulants. Such a truncation in the series should still be able to describe accurately the way in which the various thermodynamic quantities behave near $T \lesssim T_c$. Keeping only the $p = 3$ and 4 terms in the summation on the right side of (12) one obtains for Z_n

$$Z_n = \frac{d(n) \exp (- \beta J) \sqrt{n}}{\sqrt{2\pi}} \int_{-\sqrt{n}}^{\sqrt{n}} dy \exp (Cy^2) \left[1 - \frac{1}{12n} (y^4 - 6y^2 + 3) \right]. \tag{26}$$

Evaluating the integral by the saddle point method one finds the extrema at $y_0 = 0$ and

$$y_0^2 = (6C - 2) \pm (48nC^2 + 24C^2 + 4)^{1/2}/2C \tag{27}$$

It is easy to see that for $C < 0$, $y_0 = 0$ gives the maximum and for $C > 0$ the maximum is given by the larger root in (27). If C is vanishingly small $(C \to 0^+)$ but nC is finite then (27) gives $y_0^2 \approx 6nC$. For the free energy per spin $\bar{g}$, one then obtains the same expression (equation (23)) when $T > T_c$ but for $T \to T_c^-$

$$\bar{g} = - kT \ln 2 - kT \left[\tfrac{3}{4} (2J/kT - 1)^2 \right]. \tag{28}$$

This gives for the specific heat the result $(C_v/n) \rightarrow (3/2)k$ as $T \rightarrow T_c^-$. Furthermore, the spontaneous magnetization $\langle S \rangle/n$ goes to zero as $T \rightarrow T_c^-$ according to $\sqrt{3} \, (1 - T/T_c)^{1/2}$. Thus, the improved expression for $\rho(x)$ gives results in agreement with the Kac model.

Actually for this simple problem the density $\rho(S)$ is exactly known. It is given by

$$\rho(S) = \sum_{k=0}^{n} \delta \, (S + n - 2k) \binom{n}{k}. \tag{29}$$

Making use of this density one gets for Z_n the expression

$$Z_n = \frac{d(n) \exp(-\beta J)\sqrt{n}}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dy \, \{\exp(-y^2/2) \cosh(2\beta J)^{1/2} \, y\}^n, \tag{30}$$

which is exactly the same as that obtained by Kac. The point therefore of carrying out a four moment expansion of the level density for this exactly solvable model is to demonstrate that it can describe crucial thermal properties of the system adequately near the critical temperature.

5. Summary and outlook

A general statistical framework combining the usual statistical mechanics and the random matrix theory has been developed to describe disordered systems. It has been shown that, only the (Hamiltonian) ensemble-averaged level density determines the thermal properties of annealed systems whereas for the quenched systems both the average and the fluctuation properties of the spectra are important. The simple examples illustrate the use of some aspects of the moment method. The results show that a system having a Gaussian energy level density will never have any critical behaviour. The question as to what kinds of level densities lead to different types of phase transitions is an interesting one and is currently being studied. The most interesting case of a quenched system, however, has not yet been studied using the new approach. Such systems are also currently under investigation. Obviously the crucial question at this stage is, whether by applying the present method to complex ordered and disordered systems, can one obtain known results in a simpler way or obtain new results and insights. As the method appears interesting and promising we intend pursuing it to study complex systems.

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