Equivalence of replica and cavity methods for computing spectra of sparse random matrices

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We show by direct calculation that the replica and cavity methods are exactly equivalent for the spectrum of an Erdős-Rényi random graph. We introduce a variational formulation based on the cavity method and use it to find approximate solutions for the density of eigenvalues. We also use this variational method for calculating spectra of sparse covariance matrices.

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I. INTRODUCTION

Random matrix theory is a discipline with a wide range of physical applications and many beautiful mathematical results [1]. One of the aspects that makes the problem extremely complex is the fact that real physical systems are embedded in three-dimensional Euclidean space. Their Hamiltonian is often a random matrix, but the randomness is constrained in a highly nontrivial way.

The constraints are relatively less severe in the atomic nucleus, where the three dimensionality of physical space is of secondary importance. Hence the spectacular success of the early works in random matrix theory, due to Wigner [2,3] and Dyson [4]. On the other hand, the fundamental constraint arising from the two-body character of the interaction within the (model of an) atomic nucleus induces several drastic changes [5–9]. Most importantly, the density of states is not a semicircle, as suggested by Wigner, but rather it follows a Gaussian shape. Therefore, sharp band edges are missing, and Lifschitz tails develop. For the current state of the problem, see, e.g., the review [10].

An even more complicated situation arises in all random extended systems, such as disordered or amorphous semiconductors, where we must take into account the Euclidean constraints. Perhaps the easiest of these constraints is the sparsity of the Hamiltonian matrix, which is due to the finite range of interactions. If we forget the even more severe complications due to the precise number of spatial dimensions (in reality one, two, or three), we are left with the problem of determining the spectrum of a random sparse matrix.

An important breakthrough was achieved using the replica method, which was introduced in the context of random matrices in Ref. [11]. Rodgers and Bray, in their classic work [12], solved the problem in the sense that they found an integral equation for a quantity from which the density of states is readily obtained. Unfortunately, that equation still resists all attempts for an exact analytic solution. In Ref. [12], two approximative solutions were found: first, in the form of a series expansion, whose leading term coincides with the Wigner semicircle law; and, second, using a nonperturbative argument, introduced earlier in Ref. [13], the shape of the Lifschitz tails in the density of states was found.

The replica method for treating spectra of sparse matrices was further developed [14–28]. In particular, the variational formulation of the replica equations [19,20,27] enabled generating self-consistent approximations, namely, the effective medium approximation (EMA), which is analogous to the coherent potential approximation used for electrons in random potential. In these approximations, Lifschitz tails in the spectrum are absent. Further sophistication of the method consists of the single defect approximation (SDA), which obtains the Lifschitz tail in the form of an infinite sequence of delta peaks.

The complexity of the problem becomes evident when we compare these results with the density of states obtained by numerical diagonalization of large sample matrices [27,29–33]. The Lifschitz tail is smooth, while the bulk of the density of states is the combination of a continuous component with a set of delta peaks. The most marked of these peaks is at the origin, others at eigenvalues $z = \pm 1, \pm\sqrt{2}$, etc. All these structures should emerge from the solution of the Rodgers-Bray integral equation, but EMA, as well as SDA, misses all of them. The set of delta peaks was studied separately in Refs. [20,32], but a theory that would combine naturally both these peaks and the continuous component is still unavailable.

More recently, spectra of sparse matrices encoding the structure of random graphs were studied successfully using the cavity approach (see, e.g., Ref. [34]). It is based on the fact that large random graphs are locally isomorphic to trees. This was used, e.g., in Refs. [35–37] to calculate spectra of adjacency matrix and Laplacians on complex networks. In Refs. [35,36], a "self-consistent" version of SDA was used to obtain the asymptotic shape of the Lifschitz tails, which decay as a power law in the case of scale-free networks. In Ref. [37] a more sophisticated calculation led to an integral equation similar to Rodgers and Bray's [12], from which the asymptotics of Lifschitz tails is found. The cavity method provides an easy way [33] to obtain the Wigner semicircle law, as well as the Marčenko-Pastur law for a spectrum of covariance matrices. It can be also used as an efficient numerical procedure [33], reproducing all peculiarities of the density of states, including Lifschitz tails and delta peaks. The mathematical justification for the use of the cavity approach can be found in Ref. [38].

A very powerful method for computing spectral properties of random matrices is based on supersymmetry and was developed in Refs. [39,40] (see also the review [41] and a recent development in Ref. [42]). Initially, the results of replica and supersymmetric methods were found to be in conflict,

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which resulted in serious criticism of the replica trick in general [43]. The density of states of sparse random matrices was calculated using supersymmetry [44], leading to an equation that was later [45] shown equivalent to the replica result of Ref. [12]. However, the correlation of eigenvalues, which was investigated in Ref. [46] using supersymmetry for the case of sparse matrices, was not reproduced correctly in the replica method, until the integral over all saddle points was properly taken in Ref. [47]. Since then, the replica method regained its reputation as an equivalent alternative to supersymmetric methods. This was further supported by a series of papers [48–50]. Finally, let us mention the works that approach the density of states by computing the moments exactly [31,51].

In this paper, we show an alternative method to obtain the Rodgers-Bray integral equation using the cavity approach. Therefore, we prove exact equivalence of the replica and cavity methods in this case, which was previously assumed only on the basis of topological considerations for random Erdős-Rényi graphs. Moreover, as an important by-product of this proof, we present a variational formulation of the problem, which serves as a useful generator of self-consistent approximations.

II. PROJECTOR METHOD

We shall investigate the spectrum of the adjacency matrix L of an Erdős-Rényi random graph with N vertices. Therefore, the probability distribution of the matrix elements factorizes

$$\pi(L) = \prod_{i<j} [\pi_1(L_{ij})\delta(L_{ij} - L_{ji})] \prod_i \delta(L_{ii}), \tag{1}$$

where the probability density for a single off-diagonal element is

$$\pi_1(x) = \left(1 - \frac{\mu}{N}\right)\delta(x) + \frac{\mu}{N}\delta(x-1). \tag{2}$$

The key ingredient of all subsequent analysis is the resolvent:

$$R(z) = (z - L)^{-1} \tag{3}$$

and its average $\langle R(z)\rangle$ over disorder, taken with the distribution (1). It contains information on the average density of states (here we assume z on the real axis):

$$\mathcal{D}(z) = \lim_{\epsilon\to 0^+} \frac{1}{N\pi} \mathrm{Tr}\,\langle R(z - i\epsilon)\rangle. \tag{4}$$

In the spirit of the cavity method, we focus on a single vertex, surrounded by the rest of the graph. To calculate the diagonal element of the resolvent on this vertex, we use the projector method, formulated generally in Ref. [52]. For a different route that also leads to equivalent results, see Ref. [34]. Let us have an arbitrary projector P and its complement $P^C \equiv 1 - P$. Then the projected resolvent is [52]

$$PRP = \frac{P}{P(z-L)P - PLP^C \frac{P^C}{z-L} P^C L P}. \tag{5}$$

We denote the singled-out vertex as $i = 0$. Let P_0 be the projector to this vertex. Furthermore, denote $i = 1,2,\ldots,k$ neighbors of the vertex 0 on the graph represented by the matrix L and denote also a P_i projector to the neighbor i. Let us use composite indices for other vertices. If k_i is the number of neighbors of i, denote $[i,1],[i,2],\ldots,[i,k_i-1]$ as the neighbors of vertex i, except the vertex 0. The projectors to the second neighbors of 0 will be denoted using these indices, so $P_{i,i'}$ is projector on the vertex $[i,i']$. By analogy, we define the projectors to third, fourth, etc., neighbors of 0. Note that on a general graph, some of the projectors may coincide due to the presence of cycles.

The cavity approach consists of replacing the graph by a tree, which is locally isomorphic to it, i.e., neglecting all cycles on the graph. Algebraically, it is equivalent to the assumption that the complementary projectors can be written as direct sums of projectors corresponding to separate branches of the tree:

$$\begin{aligned} P_0^C &= P_{(1)} \oplus P_{(2)} \oplus \cdots \oplus P_{(k)}, \\ P_{(i)} P_i^C &= P_{(i,1)} \oplus P_{(i,2)} \oplus \cdots \oplus P_{(i,k_i-1)}, \\ P_{(i,i')} P_{i,i'}^C &= P_{(i,i',1)} \oplus P_{(i,i',2)} \oplus \cdots \oplus P_{(i,i',k_{i,i'}-1)}, \\ &\vdots \end{aligned} \tag{6}$$

where $P_{(i)}P_i = P_i$, $P_{(i,i')}P_{i,i'} = P_{i,i'}$, and so forth.

Using the projectors we define the series of scalar functions related to the resolvent:

$$\begin{aligned} g(z) &= P_0 R(z) P_0, \\ g_i(z) &= P_i \frac{{P_0}^C}{z-L} P_i, \\ g_{i,i'}(z) &= P_{i,i'} \frac{P_{(i)}\, {P_i}^C}{z-L} P_{i,i'}, \\ g_{i,i',i''}(z) &= P_{i,i',i''} \frac{P_{(i,i')}\, {P_{i,i'}}^C}{z-L} P_{i,i',i''}, \\ &\vdots \quad . \end{aligned} \tag{7}$$

From (5) and the assumptions (6) we have the chain of equations for these functions:

$$\begin{aligned} g(z) &= \frac{1}{z - \sum_{i=1}^{k} g_i(z)}, \\ g_i(z) &= \frac{1}{z - \sum_{i'=1}^{k_i-1} g_{i,i'}(z)}, \\ g_{i,i'}(z) &= \frac{1}{z - \sum_{i''=1}^{k_{i,i'}-1} g_{i,i',i''}(z)}, \\ &\vdots \quad . \end{aligned} \tag{8}$$

On a random tree, the degrees k, k_i, $k_{i,i'}$ are random variables, and therefore $g(z)$, $g_i(z)$, $g_{i,i'}(z)$, etc., are also random functions of z. To describe their properties, we define their generating functions (dependence on z becomes implicit):

$$\begin{aligned} G(\omega) &= \langle e^{-\omega\, g(z)}\rangle, \\ G_1(\omega) &= \langle e^{-\omega\, g_i(z)}\rangle, \\ G_2(\omega) &= \langle e^{-\omega\, g_{i,i'}(z)}\rangle, \\ G_3(\omega) &= \langle e^{-\omega\, g_{i,i',i''}(z)}\rangle, \\ &\vdots \quad . \end{aligned} \tag{9}$$

If the graph in question is the Erdős-Rényi random graph, all the degrees in the corresponding random tree are independent and distributed according to the Poisson distribution $P(k) = e^{-\mu}\,\mu^k/k!$. The average degree μ is the only free parameter of this model.

Calculation of the generating functions (9) is facilitated by the integral representation

$$g(z) = \frac{1}{z - \sum_{i=1}^{k} g_i(z)} = \int_0^\infty e^{-\lambda[z-\sum_{i=1}^{k} g_i(z)]}\, d\lambda \qquad (10)$$

and similarly for the other g's. Assuming for the moment that k is fixed, we get, after some algebra, the following relation between $G(\omega)$ and $G_1(\omega)$:

$$G(\omega) = 1 + \sqrt{\omega}\int_0^\infty \frac{d\lambda}{\sqrt{\lambda}}\, I_1(2\sqrt{\omega\lambda})\, e^{-\lambda z}\,[G_1(\lambda)]^k. \qquad (11)$$

Now we take into account the Poisson distribution of degrees, which gives

$$G(\omega) = 1 + \sqrt{\omega}\int_0^\infty \frac{d\lambda}{\sqrt{\lambda}}\, I_1(2\sqrt{\omega\lambda})\, e^{-\lambda z+\mu[G_1(\lambda)-1]}. \qquad (12)$$

Repeating the same steps for further generating functions we get

$$G_1(\omega) = 1 + \sqrt{\omega}\int_0^\infty \frac{d\lambda}{\sqrt{\lambda}}\, I_1(2\sqrt{\omega\lambda})\, e^{-\lambda z+\mu[G_2(\lambda)-1]}. \qquad (13)$$

Note that the form of the relation between G and G_1 is the same as between G_1 and G_2 and generally between G_m and G_{m+1} for any $m > 0$. This is due to the special property of the Poisson distribution, $kP(k)/\mu = P(k-1)$. For any other distribution this does not hold.

For an infinitely large tree we suppose that the generating functions $G_m, m = 1,2,3,\ldots$ converge to a common limit, and we can impose the condition of stationarity $G_1(\omega) = G_2(\omega)$. Therefore, we define a single function $\gamma(\omega) = G(\omega) - 1$, for which we have a closed equation:

$$\gamma(\omega) = \sqrt{\omega}\int_0^\infty \frac{d\lambda}{\sqrt{\lambda}}\, I_1(2\sqrt{\omega\lambda})\, e^{-\lambda z+\mu\gamma(\lambda)}. \qquad (14)$$

It is strictly equivalent to Eq. (18) in Ref. [12] (the Rodgers-Bray equation), which was obtained using the replica method. Hence we conclude that the explicit calculation showed the equivalence of the replica and cavity approaches in the case of the Erdős-Rényi graph, which is just the situation in which the Rodgers-Bray equation holds. Note, however, that the direct computation we used here would fail if the degree distribution was not Poissonian.

III. VARIATIONAL PROBLEM

The key result (14) can be reformulated in a different way more appropriate for approximate solution. As a first step, we define an auxiliary function $\rho(\omega) = e^{-\omega z+\mu\,\gamma(\omega)}$. Instead of the single equation (14), we can solve the pair:

$$\begin{aligned}\gamma(\omega) &= \sqrt{\omega}\int_0^\infty \frac{d\lambda}{\sqrt{\lambda}}\, I_1(2\sqrt{\omega\lambda})\,\rho(\lambda),\\ \rho(\omega) &= e^{-\omega z+\mu\,\gamma(\omega)}.\end{aligned} \qquad (15)$$

Direct solution of (15) is as difficult as solving (14). However, we can find a functional, whose stationary point is just defined by Eqs. (15). We can check explicitly that such a functional is

$$\begin{aligned}\mathcal{F}[\gamma,\rho] = &-\int_0^\infty \frac{d\omega}{\omega}\,\gamma(\omega)\rho(\omega)\\ &+\frac{1}{2}\int_0^\infty \frac{d\omega}{\sqrt{\omega}}\int_0^\infty \frac{d\lambda}{\sqrt{\lambda}}\, I_1(2\sqrt{\omega\lambda})\rho(\omega)\rho(\lambda)\\ &+\frac{1}{\mu}\int_0^\infty \frac{d\omega}{\omega} e^{-\omega z+\mu\,\gamma(\omega)}.\end{aligned} \qquad (16)$$

Note that we derived, within the cavity approach, a result that is analogous to the functional obtained in Ref. [27] using the replica trick.

The variational formulation of the problem is useful as a generator of approximations. In Ref. [20] a variational ansatz was used to derive the density of states in the EMA. Let us see now how it is obtained in our cavity procedure. If we take the exponential ansatz for the auxiliary function $\rho(\omega)$, namely,

$$\rho(\omega) = e^{-\sigma\,\omega}, \qquad (17)$$

all integrals in (16) can be performed explicitly, and we can extremalize the functional with respect to σ and $\gamma(\omega)$. In this way we find the cubic equation:

$$\sigma^3 - z\,\sigma^2 + (\mu - 1)\,\sigma + z = 0. \qquad (18)$$

It is identical to Eq. (23) in Ref. [20] obtained by the replica method. The solution can be obtained analytically, and the density of states is extracted using the formula

$$\mathcal{D}(z) = \lim_{\epsilon\to 0^+} \mathrm{Im}\frac{1}{\pi\,\sigma(z - i\epsilon)}. \qquad (19)$$

We can further improve the calculation by the following trick, which we shall refer to as the "single-shell approximation" within this paper. We may formally write the pair of Eqs. (15) as a set of four equations:

$$\begin{aligned}\gamma(\omega) &= \sqrt{\omega}\int_0^\infty \frac{d\lambda}{\sqrt{\lambda}}\, I_1(2\sqrt{\omega\lambda})\,\rho(\lambda),\\ \rho(\omega) &= e^{-\omega z+\mu\,\overline{\gamma}(\omega)},\\ \overline{\gamma}(\omega) &= \sqrt{\omega}\int_0^\infty \frac{d\lambda}{\sqrt{\lambda}}\, I_1(2\sqrt{\omega\lambda})\,\overline{\rho}(\lambda),\\ \overline{\rho}(\omega) &= e^{-\omega z+\mu\,\gamma(\omega)}.\end{aligned} \qquad (20)$$

These equations can be obtained as a condition of stationarity for the functional:

$$\begin{aligned}\mathcal{F}_1[\gamma,\rho,\overline{\gamma},\overline{\rho}] = &-\int_0^\infty \frac{d\omega}{\omega}[\gamma(\omega)\overline{\rho}(\omega) + \overline{\gamma}(\omega)\rho(\omega)]\\ &+\int_0^\infty \frac{d\omega}{\sqrt{\omega}}\int_0^\infty \frac{d\lambda}{\sqrt{\lambda}}\, I_1(2\sqrt{\omega\lambda})\rho(\omega)\overline{\rho}(\lambda)\\ &+\frac{1}{\mu}\int_0^\infty \frac{d\omega}{\omega} e^{-\omega z}(e^{\mu\,\gamma(\omega)} + e^{\mu\,\overline{\gamma}(\omega)}).\end{aligned} \qquad (21)$$

If Eqs. (20) were solved exactly, we would have $\gamma(\omega) = \overline{\gamma}(\omega)$ and $\rho(\omega) = \overline{\rho}(\omega)$. The same also would hold in the case of the effective medium approximation, which amounts to taking the ansatz $\rho(\omega) = \overline{\rho}(\omega) = e^{-\sigma\,\omega}$, so apparently the set (20) does not bring any advantage over (15). However, relaxing

the condition $\rho(\omega) = \overline{\rho}(\omega)$ we can get an improvement in an approximate solution. Indeed, we can take the ansatz

$$\rho(\omega) = e^{-\sigma\,\omega} \tag{22}$$

as in EMA but allow $\overline{\rho}(\omega)$ to adjust itself freely so that $\mathcal{F}_1$ is stationary. In this way we introduce an error, because $\rho(\omega) \neq \overline{\rho}(\omega)$ and $\gamma(\omega) \neq \overline{\gamma}(\omega)$, but we gain a better approximation for the density of states.

After some algebra, we get the following equation for the quantity $\tau = z\,\sigma$:

$$z^2 = \mu + \tau + e^{-\mu} \sum_{l=1}^{\infty} \frac{\mu^l}{(l-1)!}\,\frac{l}{\tau - l}. \tag{23}$$

The fact that the equation depends on z^2 means that the spectrum is symmetric with respect to the point $z = 0$. For a general z on the real axis, Eq. (23) can be easily solved numerically. We find that there are at most two roots with nonzero imaginary parts (complex conjugate to each other). Those values of z for which all solutions are real correspond to gaps in the spectrum. The general picture is that there is a very narrow gap around $z = 0$, separating two halves of a wide band, containing most of the eigenvalues. We can call this band (not quite precisely) the "bulk" of the density of states.

In the middle of the bulk, there is a δ-function contribution just at $z = 0$, whose weight can be found exactly and is equal to $e^{-\mu}$. On both sides of the bulk, there are a series of small side bands separated by gaps. The density of states therefore has the form

$$\mathcal{D}(z) = e^{-\mu}\delta(z) + \mathcal{D}_c(z), \tag{24}$$

where $\mathcal{D}_c(z)$ is a continuous function. The interpretation of the δ-function is straightforward. It corresponds to single isolated vertices, whose fraction is just equal to $e^{-\mu}$, and they all contribute with the same eigenvalue 0.

Some analytical information on the continuous part $\mathcal{D}_c(z)$ can be found from an approximate solution of Eq. (23). For $e^{-\mu} \ll 1$ we can find approximately the edge of the gap around $z = 0$. We get

$$\mathcal{D}_c(z) \simeq \frac{1}{2\pi\,z}\sqrt{4\psi(\mu)\,z^2 - e^{-2\mu}}, \tag{25}$$

where we denote

$$\psi(\mu) = e^{-\mu} \sum_{l=1}^{\infty} \frac{\mu^l}{l!\,l} = \mu\,e^{-\mu}\,{}_2F_2(1,1;2,2;\mu). \tag{26}$$

We can see that the gap edge is at $z_0 = \frac{1}{2}e^{-\mu}/\sqrt{\psi(\mu)}$.

For the tails, we can calculate analytically the side bands in an approximation that becomes exact for $|z| \to \infty$. The computation goes as follows. Each of the side bands can be identified with one term in the infinite sum over l in (23). The tails of the spectrum corresponding to large $|z|$ are identified with large l. In the crudest approximation, the solution is $\tau \simeq l$. Therefore, we introduce a new variable η by $\tau = l + \eta$. So (23) assumes the form

$$z^2 = \mu + l + \eta + e^{-\mu}\frac{\mu^l}{(l-1)!}\,\frac{l}{\eta} + e^{-\mu}\sum_{l'=1(l'\neq l)}^{\infty} \frac{\mu^{l'}}{(l'-1)!}\,\frac{l'}{l - l' - \eta}. \tag{27}$$

For large l we can expand the infinite series in powers of η and keep only the lowest terms, so

$$z^2 = \mu + \Delta_l(\mu) + l + [1 - \Gamma_l(\mu)]\,\eta + e^{-\mu}\frac{\mu^l}{(l-1)!}\,\frac{l}{\eta} + O(\eta^2), \tag{28}$$

where

$$\Delta_l(\mu) = e^{-\mu}\sum_{l'=1(l'\neq l)}^{\infty} \frac{\mu^{l'}}{(l'-1)!}\,\frac{l'}{l - l'}, \qquad \Gamma_l(\mu) = e^{-\mu}\sum_{l'=1(l'\neq l)}^{\infty} \frac{\mu^{l'}}{(l'-1)!}\,\frac{l'}{(l - l')^2}. \tag{29}$$

So, for each l large enough, we have two "bubbles" of a nonzero density of states. The two bubbles are symmetric to each other with respect to the origin. The "bubbles" are separated by gaps, so each "bubble" has well-defined lower and upper edges, z_{l-} and z_{l+}, respectively. For large l the approximate form of the "bubble" is given by the solution of a quadratic equation in η, so

$$\mathcal{D}_l(z) \simeq \frac{|z|}{\pi}\left\{[1 - \Gamma_l(\mu)]\frac{e^{-\mu}\,l\,\mu^l}{(l-1)!} - \left[\frac{z^2 - \mu - l - \Delta_l(\mu)}{2}\right]^2\right\}^{1/2} \times \left\{\frac{e^{-\mu}\,l\,\mu^l}{(l-1)!} + (z^2 - \mu - l)l + [1 - \Gamma_l(\mu)](l)^2\right\}^{-1}. \tag{30}$$

The width of the bubble $z_{l+} - z_{l-}$ approaches zero for $l \to \infty$. This justifies considering η as a small parameter in the expansion (28). For large l the "bubbles" have a semicircle shape, and their weight is

$$W_l = \int_{z_{l-}}^{z_{l+}} \mathcal{D}_l(z)\,dz \simeq \frac{1}{2}\,e^{-\mu}\,\frac{\mu^l}{l!}. \tag{31}$$

We recognize the Poisson distribution with mean μ. This reflects the Poisson distribution of degrees of the random graph. The factor $1/2$ stems from the fact that we have two bubbles for each l. The center of the bubble corresponding to l is at $z_l = \sqrt{l + \mu + \Delta_l(\mu)}$; thus the distance between two successive bubbles is $\Delta z_l \simeq (4z_l)^{-1/2}$. Hence we deduce the approximate density of states in the tails, for $|z| \to \infty$:

$$\mathcal{D}_{\rm tail}(z) \simeq \frac{e^{-\mu}\,|z|\,\mu^{z^2}}{\Gamma(z^2 - 1)} \simeq \frac{e^{-\mu}}{\sqrt{2\pi}}\left(\frac{e\mu}{z^2}\right)^{z^2}. \tag{32}$$

This is the shape of the Lifschitz tail, which was already obtained by Refs. [12] and [20].

To assess the quality of the approximations used, we compare the results arising from EMA [Eq. (18)], from the single-defect [20,33], and single-shell [Eq. (23)] approximations with an average density of states obtained by numerical diagonalization of sample matrices. In Fig. 1 we can see the

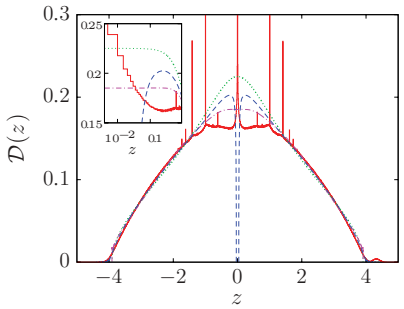

FIG. 1. (Color online) Density of states for the adjacency matrix of an Erdős-Rényi graph, with average degree $\mu = 3$. The solid line shows the result of the numerical diagonalization of a matrix of size $N = 1000$, averaged over 75 000 random realizations. The dotted line is the result of an effective medium approximation, the dot-dashed line is the single-defect approximation, and the dashed line is the single-shell approximation. In the inset, a detail of the density of states around the center of the band is plotted in semilogarithmic scale.

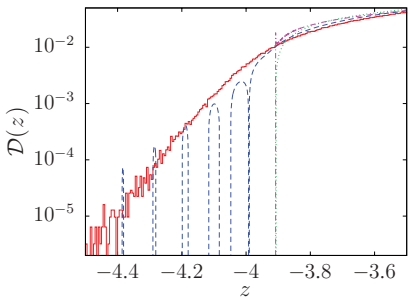

FIG. 2. (Color online) The detail of the left tail of the density of states shown in Fig. 1. The solid line shows the result of numerical diagonalization, the dotted line is the result of effective medium approximation, the dot-dashed line is the single-defect approximation, and the dashed line is the single-shell approximation.

spectrum for $\mu = 3$ and matrices of size $N = 1000$ averaged over 75 000 realizations. We can clearly identify the delta peaks, as well as the complicated shape of the continuous part of the spectrum near the center of the bulk. Interestingly, both EMA and the single-shell approximations are very good if we are neither close to the center nor at the tails of the spectrum. Close to the center, the shape of the density of states is rather complex, as shown in the inset in Fig. 1. There is a shallow depression, followed by a divergence at $z = 0$. The form of the singularity at $z = 0$ seems to be close to a logarithmic divergence, although the data do not provide decisive evidence. None of the three approximations reproduce this singularity. EMA and SDA are constant around $z = 0$, while the single-shell approximation exaggerates the depression around $z = 0$ to such an extent that a spurious gap is created. This is an artifact of the approximation. However, the delta peak at the origin is, correctly, present in the single-shell approximation.

A similar comparison also was done at the tail of the density of states. We can see in Fig. 2 a detail of the same data as shown in Fig. 1. Note that, for any finite N, the density of states is not mirror symmetric with respect to the line $z = 0$, because the average value of the off-diagonal elements of the matrix L is strictly positive. Only in the limit $N \to \infty$ does the spectrum become symmetric. The single largest eigenvalue is split off the rest of the spectrum [53], and the small bump in the positive tail corresponds to this effect. In the limit $N \to \infty$ this bump would vanish, as the weight of the single largest eigenvalue becomes negligible compared to the rest of the spectrum.

As shown in Fig. 2, we can see that the single-shell approximation is superior to both EMA and SDA in the tail region, from two aspects. First, the spurious band edge of EMA and SDA is shifted toward larger $|z|$, so that the interval in which $\mathcal{D}(z)$ is well reproduced is wider. Second, the single-shell approximation also displays nonzero density of states in some regions of the Lifschitz tails, although, instead of exhibiting a smooth behavior everywhere, the density of states is concentrated in "bubbles." The gaps separating the "bubbles" are again artifacts of the approximation, to the same extent as the sharp band edge is an artifact of EMA and SDA. On the other hand, it is an important improvement over SDA [20]. The delta peaks of SDA are widened into continuous bands in our approach. In fact, this is to be expected, because the single-shell approximation can be rightly interpreted as a self-consistent version of SDA. Therefore, it should be better than SDA in principle, although this *a priori* judgment may turn out to be incorrect in practice, as the single-shell approximation is better than SDA sometimes (in the tail) but worse elsewhere (around $z = 0$).

Finally, let us note that similar "bubbles" at the tails were also seen in approximations derived using the replica method by Ref. [21] for the Laplacian of a random graph and by Ref. [25] for sparse covariance matrices.

IV. COVARIANCE MATRICES

Another application of the method presented here is investigation of sparse covariance matrices. They can be considered as arising from a bipartite graph where edges connect vertices from the set A with vertices from the set B. We denote the size of the sets N_A and N_B, respectively. In the thermodynamic limit, $N_A \to \infty$, $N_B \to \infty$, we fix the ratio $\alpha = N_A/N_B$ constant. In the bipartite analog of an Erdős-Rényi random graph, the degrees of vertices in A and B follow Poisson distributions with average degree μ_A and μ_B, respectively, where $\mu_B/\mu_A = \alpha$. The problem has a long history, starting with the work of Marčenko and Pastur [54], and was investigated recently by the replica method in Ref. [25].

The adjacency matrix of the bipartite graph has the form

$$L = \begin{pmatrix} 0 & M^T \\ M & 0 \end{pmatrix}, \tag{33}$$

where the first block of indices corresponds to set A, and the second block to set B. We define the contraction, or covariance, matrix $C_A = M^T M$, which acts solely in the set A (and similarly $C_B = M M^T$, which acts solely in the set B). The spectra of the matrices L, C_A, and C_B are closely related. We define $\mathcal{D}_A(z) = \lim_{\epsilon \to 0^+} \mathrm{Im} \sum_{i \in A} [(z - i\epsilon - L)^{-1}]_{ii}/(N_A \pi)$ as the partial density of states of L

restricted to the set A and $\mathcal{D}_{CA}(z) = \lim_{\epsilon\to 0^+} \mathrm{Im} \sum_{i\in A}[(z - i\epsilon - C_A)^{-1}]_{ii}/(N_A\,\pi)$ as the density of states of the correlation matrix C_A. It can be easily shown that

$$\mathcal{D}_{CA}(z) = \frac{1}{\sqrt{z}}\mathcal{D}_A(\sqrt{z}). \tag{34}$$

This relation remains in force also after averaging over the randomness in the matrix M. Therefore, to calculate the average density of states of the covariance matrix C_A it is enough to investigate the matrix element $\langle[(z - L)^{-1}]_{ii}\rangle$ for any $i \in A$. To this end, we define the generating functions

$$\begin{aligned} \gamma_A &= \langle e^{-\omega[(z-L)^{-1}]_{ii}}\rangle - 1 \text{ for } i \in A, \\ \gamma_B &= \langle e^{-\omega[(z-L)^{-1}]_{jj}}\rangle - 1 \text{ for } j \in B. \end{aligned} \tag{35}$$

The further procedure follows closely that of the previous section. Finally, we get a set of four coupled equations, very similar to the set we encountered in the single-shell approximation:

$$\begin{aligned} \gamma_A(\omega) &= \sqrt{\omega}\int_0^\infty \frac{d\lambda}{\sqrt{\lambda}}\, I_1(2\sqrt{\omega\lambda})\,\rho_B(\lambda), \\ \rho_B(\omega) &= e^{-\omega z + \mu_A\,\gamma_B(\omega)}, \\ \gamma_B(\omega) &= \sqrt{\omega}\int_0^\infty \frac{d\lambda}{\sqrt{\lambda}}\, I_1(2\sqrt{\omega\lambda})\,\rho_A(\lambda), \\ \rho_A(\omega) &= e^{-\omega z + \mu_B\,\gamma_A(\omega)}. \end{aligned} \tag{36}$$

We can easily check that the solution of these equations makes the following functional stationary:

$$\begin{aligned} &\mathcal{F}_{AB}[\gamma_A,\rho_A,\gamma_B,\rho_B] \\ &\quad= -\int_0^\infty \frac{d\omega}{\omega}\,[\gamma_A(\omega)\rho_A(\omega) + \gamma_B(\omega)\rho_B(\omega)] \\ &\qquad+ \int_0^\infty \frac{d\omega}{\sqrt{\omega}}\int_0^\infty \frac{d\lambda}{\sqrt{\lambda}}\, I_1(2\sqrt{\omega\lambda})\rho_A(\omega)\rho_B(\lambda) \\ &\qquad+ \int_0^\infty \frac{d\omega}{\omega} e^{-\omega z}\left(\frac{1}{\mu_A}\, e^{\mu_A\,\gamma_B(\omega)} + \frac{1}{\mu_B}\, e^{\mu_B\,\gamma_A(\omega)}\right). \end{aligned} \tag{37}$$

For an approximate solution of Eqs. (36) we use again a variational ansatz. In analogy with EMA, we assume the following form:

$$\begin{aligned} \rho_A(\omega) &= e^{-\sigma_A\,\omega}, \\ \rho_B(\omega) &= e^{-\sigma_B\,\omega}. \end{aligned} \tag{38}$$

The insertion of (38) in (37) produces finally two uncoupled cubic equations for σ_A and σ_B. The equation relevant for us is

$$\begin{aligned} &z\,\sigma_B^3 + [(1-\alpha)\mu_A + \alpha - 1 - z^2]\,\sigma_B^2 \\ &\quad+ (\mu_A\,\alpha + 1 - 2\alpha)\,z\,\sigma_B + z^2\,\alpha = 0, \end{aligned} \tag{39}$$

where we used $\alpha = \mu_B/\mu_A$. The average density of states for the covariance matrix C_A is found considering the first equation of (36) and the relation (34); thus

$$\mathcal{D}_{CA}(z) = \frac{1}{\pi\sqrt{z}} \lim_{\epsilon\to 0+} \mathrm{Im}\frac{1}{\sigma_B(\sqrt{z} - i\epsilon)}. \tag{40}$$

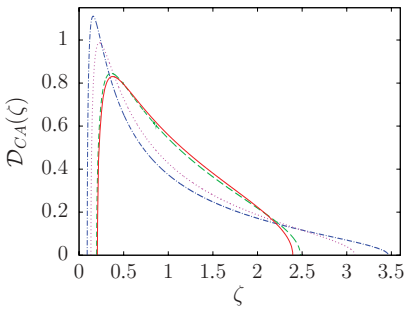

FIG. 3. (Color online) Density of states for the correlation matrix based on a sparse adjacency matrix, for $\alpha = 0.3$. The average degree is $\mu_A = 3$ (dash-dotted line), 5 (dotted line), and 50 (dashed line). The full line is the Marčenko-Pastur density (41), i.e., the limit $\mu_A \to \infty$.

The solution can be obtained analytically, but we shall not show the formula here. However, we can check that in the limit $\mu_A \to \infty$ with α and $\zeta = z/\mu_A$ fixed we get

$$\mathcal{D}_{CA}(\zeta) = \frac{1}{2\pi\,\alpha\,\zeta}\sqrt{[(1+\sqrt{\alpha})^2 - \zeta][\zeta - (1-\sqrt{\alpha})^2]}, \tag{41}$$

which is the Marčenko-Pastur (MP) density of states [54].

In Fig. 3 we show the density of states as function of $\zeta = z/\mu_A$ for several values of μ_A, as found by the solution of (39). We can see that the approach to MP density is rather slow. We found that the difference can be considered small only at about $\mu_A \simeq 50$.

V. CONCLUSIONS

We considered a random graph of large size $N \to \infty$ of two types: first, a "classical" Erdős-Rényi graph, and, second, a random bipartite graph. We calculated the density of eigenvalues for adjacency matrices of these graphs. In the case of the bipartite graph, the final result was the density of states of the covariance matrix, defined by a contraction of the adjacency matrix.

Our contribution to the problem of spectra of sparse random matrices consists of showing that the cavity approach, i.e., approximation of the random graph by a random tree, is exactly equivalent to the calculation by the replica method in the thermodynamic limit. Furthermore, we demonstrated how the cavity calculation can be formulated as a variational problem, similar to but substantially simpler than the variational formulation arising from the replica method. At minimum, we do not need to consider the possibility of replica-breaking solutions, which are known to exist and contribute to the finite-size corrections [47]. We can interpret it also in the following manner. Since we are working directly with an infinite-size system, $N = \infty$, the physics behind the replica-breaking states has no effect.

The variational formulation introduced here is a very practical starting point for approximations. The exponential ansatz leads to results identical to the effective-medium approximation studied earlier [20]. However, using our variational scheme, the approximation can be easily improved by what we call a "single-shell approximation." It produces the Lifschitz tail in the density of states in the form of a series of "bubbles." We are able to calculate the weight and distance of

the bubbles. Hence we arrive at average density of states in the tail, which is identical to the result of Rodgers and Bray [12]. Furthermore, we applied the method also to the spectra of sparse covariance matrices, where we easily derived a formula generalizing the Marčenko-Pastur density of states.

The variational formulation introduced here can be used not only as a generator of approximations, but also as a basis of numerical methods. Indeed, there is no principal obstacle for numerical extremalization of the functional of two variables. This contrasts with the variational methods based on the replica trick, where the replica limit $n \to 0$, involving analytic continuation, must be done after extremalization, which makes the method numerically unfeasible.

We believe that the method can also be applied for other types of random graphs. We must, however, admit a serious limitation of our method, which is the Poisson distribution of degrees of the graph. Therefore, it is, for example, not applicable directly for graphs with a power-law degree distribution. We believe that the roots of this limitation lie quite deep. For example, to the best of our knowledge, there is no replica calculation available for random graphs defined by their degree sequence only. On the other hand, there are no results from the cavity method for those random graphs with a power-law degree distribution, for which replica calculations do exist, like those of Ref. [23]. The point is, that for a Erdős-Rényi graph, it is well established that the local topology is isomorphic to a random tree. For a graph with a general degree sequence, not obeying Poisson statistics, this may or may not be true. The question of equivalence or not of the replica and cavity methods is intimately related to the question of local isomorphism to a tree, which is rather complex and not solved in general. Hence, a successful treatment of such cases by both the replica and cavity methods in parallel would require, very probably, completely novel ideas.

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