

## Spectra of random graphs with arbitrary expected degrees

Raj Rao Nadakuditi<sup>1</sup> and M. E. J. Newman<sup>2</sup>

<sup>1</sup>*Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Michigan 48109, USA*

<sup>2</sup>*Department of Physics and Center for the Study of Complex Systems, University of Michigan, Ann Arbor, Michigan 48109, USA*

(Received 13 August 2012; published 10 January 2013)

We study random graphs with arbitrary distributions of expected degree and derive expressions for the spectra of their adjacency and modularity matrices. We give a complete prescription for calculating the spectra that is exact in the limit of large network size and large vertex degrees. We also study the effect on the spectra of hubs in the network, vertices of unusually high degree, and show that these produce isolated eigenvalues outside the main spectral band, akin to impurity states in condensed matter systems, with accompanying eigenvectors that are strongly localized around the hubs. We give numerical results that confirm our analytic expressions.

DOI: [10.1103/PhysRevE.87.012803](https://doi.org/10.1103/PhysRevE.87.012803)

PACS number(s): 89.75.Hc, 02.70.Hm, 64.60.aq

### I. INTRODUCTION

The topology of complex networks, such as social, biological, and technological networks, can be represented in matrix form using an adjacency matrix or any of several other related matrices such as the graph Laplacian or the modularity matrix [1,2]. The spectral properties of these matrices—their eigenvalues and eigenvectors—are related to a range of network features of scientific interest, including optimal partitions [3,4], percolation properties [5], community structure [6,7], and the behavior of network dynamical processes such as random walks, current flow, diffusion, and synchronization [8,9]. As a result, the study of network spectra has been the subject of considerable research effort for some years. This effort has taken a number of forms. One has been the study of the spectra of empirically observed networks, which can be calculated by numerical means for networks of size up to hundreds of thousands of vertices [8,10]. Another, which is the topic of this paper, is the study of the spectra of model networks. A fundamental question we would like to answer is how particular structural features of networks are reflected in network spectra, and model networks provide an ideal setting in which to investigate this question.

Some results in this area have been known for a long time. For example, the very simplest of network models, the Poisson random graph, studied as far back as the 1950s by Erdős, Rényi, and others [11,12], has a symmetric adjacency matrix whose elements are independent identically distributed random variables. Such matrices are known, subject to some conditions but regardless of the precise distribution of their elements, to have a universal spectrum obeying the Wigner semicircle law and eigenvectors that are distributed isotropically at random, except for the leading eigenvalue and eigenvector, whose values are governed by the Perron-Frobenius theorem and the average degree of the network [13–20].

As we have come to understand in the past decade, however, the random graph is a poor model for the structure of real-world networks. In particular, the frequency distribution of the degrees of vertices in the random graph is Poissonian, while the degree distribution of most real-world networks is highly right-skewed, often having a power-law or exponential tail of “hubs” with degree far above the mean. Luckily, it turns out to be possible to create generalizations of the basic random graph that incorporate arbitrary degree distributions, including

skewed distributions, the best-known such model being the so-called configuration model [21,22]. The configuration model is solvable exactly for many of its structural properties, including its complete component structure [22–24] and percolation properties [25,26], and the results have led us to a better understanding of the profound effect the degree distribution has on network topology.

In this paper we study the spectral properties of the configuration model. Motivated by recent developments in random matrix theory, we derive a simple recipe for calculating the spectrum of the adjacency matrix of the model. We show that the spectrum is composed of three fundamental elements, all of which have clear correlates in the structure of the network. The elements are (1) the leading eigenvalue, which is dictated primarily by the average network degree; (2) a continuous band or “bulk spectrum,” analogous to the Wigner semicircle but taking a different shape; and (3) in some but not all cases, additional eigenvalues outside of the continuous band which correspond to the hubs in the network and which have eigenvectors that are strongly localized about those hubs.

In addition to our analytic developments, we also confirm the form and behavior of each of these elements with numerical calculations on example networks generated using the configuration model.

A number of previous authors have examined the spectral properties of the configuration model. Farkas *et al.* [10] performed numerical calculations on large samples generated using the model and demonstrated that there are clear deviations from the semicircle law for non-Poisson choices of the degree distribution and especially for power-law distributions. Dorogovtsev *et al.* [27] gave an analytic route to the full spectrum, though their method is complex, involving the solution of a nonlinear integral equation containing Bessel functions, which at present can only be done approximately. Kühn [28] has given a different analytic treatment that is exact when vertex degrees are finite, which is the opposite of the limit of large degrees that we treat in this paper. Chung *et al.* [29] gave a rigorous derivation of the expected value of the largest eigenvalue in the spectrum in the limit of a dense network. Our calculations extend these studies by providing a simple derivation of the full spectrum which is exact in the limit of large vertex degrees and confirms earlier findings while shedding new light on features of the spectrum and their implications for network structure.

**II. THE MODEL**

In this paper, we study the spectral properties of the configuration model—or, more precisely, a slight variant of the model, as we now describe.

The configuration model is a model of an undirected random graph with a specified number of vertices  $n$  and a given degree sequence. In this model one first specifies a degree sequence, meaning one specifies the degree of each of the  $n$  vertices. Let the degree of vertex  $i$  be denoted  $k_i$  and let us visualize the degree as  $k_i$  ends or “stubs” of edges emerging from the vertex. Then the configuration model is defined as the ensemble of pairwise matchings of stubs in which every matching appears with equal probability. That is, a configuration model network with the given degree sequence is generated by repeatedly choosing two stubs uniformly at random from those available and joining them together to form a complete edge. This process continues until all stubs have been joined and no unattached stubs remain. (For this to work, the number of stubs must be even, and hence the model is defined only for degree sequences whose sum  $\sum_i k_i$  is even.)

The configuration model provides a way to generate networks that have any degree sequence we desire while being essentially random in other respects—there are no correlations or long-range structure in the configuration model ensemble.

A crucial feature of the configuration model for our purposes will be the expected number of edges between a vertex pair. It is straightforward to show, given the degree sequence, that the expected number of edges between vertices  $i$  and  $j$  is equal to  $k_i k_j / 2m$  in the limit of large network size, where  $m = \frac{1}{2} \sum_i k_i$  is the number of edges in the network. Note that it is possible to generate networks with multiedges—pairs of vertices connected by more than one parallel edge. The actual number of edges between vertices  $i$  and  $j$  is multinomially distributed with mean  $k_i k_j / 2m$ .

However, edges in the configuration model are not statistically independent. Since the degrees of vertices are fixed, the presence of an edge from vertex  $i$  to vertex  $j$  makes it less likely that there will be an edge from  $i$  to any other vertex, and hence edges that share a common end are correlated. When the degree is large, the correlations become small and the multinomial distribution of edge number becomes approximately Poisson, but for networks with finite average degree the correlations will always be present and may be significant.

These correlations make analysis of the model more difficult and so in this paper we consider a modified model in which the number of edges between each pair of vertices is *defined* to be an independent random variable with mean  $k_i k_j / 2m$  and value drawn from a Poisson distribution with that mean. In this model,  $k_i$  becomes the expected degree of vertex  $i$  and  $m$  is the expected total number of edges. When degrees become large, which is the primary regime that we consider in this paper, the actual degrees will be narrowly peaked about their expected values, so the properties of the variant model and the standard configuration model, including the spectral properties that we study, become the same. This model (or slight variants of it) has been studied previously by a number of authors, notably Chung and Lu [30], with whose work it is perhaps most strongly associated.

In this paper we consider networks in the limit of large size  $n$  with expected vertex degrees drawn from a fixed probability density  $p(k)$ , so that  $p(k) dk$  is the fraction of vertices with expected degree in the interval from  $k$  to  $k + dk$ . (Note that the expected degree need not be an integer, although one is free to choose it to have integer values if one wishes.) More precisely, we consider a sequence of networks of increasing size with fixed expected degrees  $k_i$  and additional degrees drawn from  $p(k)$  as  $n$  becomes larger. Thus for finite  $n$  the expected degree of any particular vertex  $i$  remains constant as  $n$  becomes large and the empirical degree distribution converges to  $p(k)$  in the large- $n$  limit.

The adjacency matrix  $\mathbf{A}$  of a network generated according to this model is the  $n \times n$  symmetric matrix with integer elements  $A_{ij}$  equal to the number of edges between vertices  $i$  and  $j$ . Our primary goal in this paper is to calculate the average spectrum of the adjacency matrix within the model ensemble, which we do in two stages. We write the matrix as

$$\mathbf{A} = \langle \mathbf{A} \rangle + \mathbf{B}, \tag{1}$$

where  $\langle \mathbf{A} \rangle$  is the ensemble average of  $\mathbf{A}$ , which has elements  $\langle A_{ij} \rangle = k_i k_j / 2m$ , and  $\mathbf{B}$  is the deviation from that average. Our approach is first to calculate the spectrum of the matrix  $\mathbf{B}$ , whose elements are, by definition, independent random variables with zero mean, although crucially they are not identically distributed. Once we have the spectrum of  $\mathbf{B}$ , then the spectrum of  $\mathbf{A}$  is calculated from it in a separate step.

The matrix  $\mathbf{B}$  has elements

$$B_{ij} = A_{ij} - \langle A_{ij} \rangle = A_{ij} - \frac{k_i k_j}{2m} \tag{2}$$

and is of interest in its own right. It is known as the modularity matrix and forms the basis for one of the most widely used methods for detecting modules or communities in networks [6,7]. The methods described in this paper thus give us the spectrum of both the adjacency matrix and the modularity matrix.

Note that the elements of the modularity matrix have the same variance as the corresponding elements of the adjacency matrix which, since they are Poisson distributed, have variance equal to their mean  $k_i k_j / 2m$ . Hence,

$$\langle B_{ij}^2 \rangle = \frac{k_i k_j}{2m}, \tag{3}$$

which will be important shortly.

**III. SPECTRUM OF THE MODULARITY MATRIX**

As discussed in the previous section, we will first calculate the spectrum of the modularity matrix  $\mathbf{B}$ , defined by Eq. (2), and then calculate the spectrum of the adjacency matrix from it in a separate step. We begin by developing some fundamental notions concerning random variables that will be important for our derivations.

Suppose we have two independent random variables,  $x$  and  $y$ , ordinary scalar variables, with probability densities  $p_x(x)$  and  $p_y(y)$ . What is the probability that their sum  $x + y$  will have a particular value  $z$ ? The answer to this question is well known and simple. The probability density

for  $z$  is

$$\begin{aligned} p(z) &= \iint p_x(x)p_y(y)\delta(x+y-z) dx dy \\ &= \int p_x(x)p_y(z-x) dx, \end{aligned} \quad (4)$$

which is the convolution of the two distributions. Similarly, we can ask for the probability that the product  $xy$  has value  $z$ , which is given by the multiplicative convolution

$$\begin{aligned} p(z) &= \iint p_x(x)p_y(y)\delta(xy-z) dx dy \\ &= \int p_x(x)p_y(z/x) \frac{dx}{x}. \end{aligned} \quad (5)$$

A scalar random variable can be thought of as the single eigenvalue of a  $1 \times 1$  random matrix. A  $1 \times 1$  matrix is diagonal by definition and its one eigenvalue is trivially equal to its one element. A natural generalization of the convolution results above is to ask what their equivalent is for larger random matrices,  $2 \times 2$ ,  $3 \times 3$ , and so forth, where we will confine ourselves to symmetric matrices so the eigenvalues are real. That is, if we know the probability density of the eigenvalues—the so-called spectral density—of two independent symmetric random matrices, what is the spectral density of their sum or product? The answer is no longer a simple convolution, because matrices do not in general commute, so what is the appropriate generalization? Unfortunately, this question does not have a straightforward answer because it turns out that a knowledge of the spectral densities alone is not enough. In general, one needs to know the distribution of the entire matrices to calculate the spectral density of their sum or product. There is, however, one case in which relatively simple results apply, which is when the eigenvectors of the two matrices are themselves random and uncorrelated.

Recall that the eigenvectors of a symmetric matrix are orthogonal—for an  $n \times n$  matrix they define a set of orthogonal axes in an  $n$ -dimensional vector space. Thus, if we have two random symmetric matrices, the eigenvectors of one can always be transformed into the eigenvectors of the other by a suitable rotation and/or reflection—in other words by a suitable orthogonal transformation. If for different choices of the random matrices the transformations needed to do this are distributed isotropically—essentially if all possible such transformations are equally likely—then the random matrices are said to be *free*. Loosely, one can say that two random matrices are free if the angle between their eigenvectors is also random. The mathematics of free random variables has been developed extensively since the 1990s and is known by the name of *free probability theory* [31].

The crucial observation now is the following: For free matrices the spectral density of their sum or product is a function only of the individual spectral densities. It turns out that one no longer needs to know the entire distribution of the matrices themselves and well-defined generalizations of the convolution equations, Eqs. (4) and (5), exist. For the sum of two matrices the appropriate generalization is known as the *free convolution* or *free additive convolution*; for the product of matrices it is the *free multiplicative convolution*. Thus, if two symmetric random matrices have spectral densities  $p_x(x)$

and  $p_y(y)$ , then the spectral density of their product is the free multiplicative convolution

$$p(z) = (p_x \boxtimes p_y)(z), \quad (6)$$

where  $\boxtimes$  denotes the convolution. Although this defines the convolution in principle, it does not tell us how to calculate it. We will come to that in a moment, but first let us return to the configuration model and see why this is a useful result.

We wish to calculate the spectral density of the modularity matrix  $\mathbf{B}$ , which for an undirected network is a symmetric random matrix whose elements have zero mean but different variances, equal to  $k_i k_j / 2m$ —see Eq. (3). Let us define a normalized modularity matrix  $\tilde{\mathbf{B}}$  by

$$\tilde{\mathbf{B}} = \mathbf{D}^{-1/2} \mathbf{B} \mathbf{D}^{-1/2}, \quad (7)$$

where  $\mathbf{D}$  is the diagonal matrix with elements  $k_i$ .  $\tilde{\mathbf{B}}$  has elements  $\tilde{B}_{ij} = B_{ij} / \sqrt{k_i k_j}$ , so each is divided by a factor proportional to its standard deviation and hence, though not identically distributed, all elements now have the same variance, equal to  $1/2m$ . So long as the vertex degrees are large, matrices with this property are known to have an eigenvector basis oriented isotropically at random and to have spectral density obeying the Wigner semicircle law [13–20], which, for our particular matrix, takes the form

$$\rho_c(z) = \frac{1}{2\pi} \sqrt{4c - c^2 z^2}, \quad (8)$$

where  $c = 2m/n$  is the average degree in the network. The requirement that vertex degrees be large is necessary because deviations from the semicircle law are known to arise for very sparse matrices [32]. For small degrees, therefore, the results given here will only be approximate.

Now consider an eigenvalue  $z$  of the modularity matrix  $\mathbf{B}$  itself, satisfying  $\mathbf{B}\mathbf{b} = z\mathbf{b}$ , where  $\mathbf{b}$  is the corresponding eigenvector. Multiplying by  $\mathbf{D}^{1/2}$ , writing  $\tilde{\mathbf{B}} = \mathbf{D}^{1/2} \mathbf{B} \mathbf{D}^{1/2}$ , and defining  $\mathbf{v} = \mathbf{D}^{1/2} \mathbf{b}$ , this can also be written

$$\tilde{\mathbf{D}} \tilde{\mathbf{B}} \mathbf{v} = z \mathbf{v}. \quad (9)$$

In other words, the modularity matrix has the same eigenvalues as the matrix  $\tilde{\mathbf{D}} \tilde{\mathbf{B}}$ , which is the product of the diagonal matrix  $\tilde{\mathbf{D}}$ , which, by definition, has spectral density equal to the degree distribution  $p(k)$  and the symmetric matrix  $\tilde{\mathbf{B}}$ , with spectral density  $\rho_c(z)$  given by Eq. (8).

But it is precisely to the products of such random matrices that Eq. (6) relates, and, hence, applying that equation, we arrive at the principal result of this paper: The spectral density of the modularity matrix for a network with arbitrary expected degrees is equal to the free multiplicative convolution of the degree distribution with the Wigner semicircle. That is, the spectral density  $\rho(z)$  is given by

$$\rho(z) = (p \boxtimes \rho_c)(z), \quad (10)$$

where  $p(k)$  is the distribution of expected degrees and  $\rho_c(z)$  is given by Eq. (8).

This result is of immediate practical utility. Numerical methods exist for computing free multiplicative convolutions efficiently [33,34], which means we can use existing numerical packages to compute spectral densities easily and rapidly for a wide range of degree distributions.

For the purposes of the present paper, however, we would like to know more. In particular, we would like explicit formulas for calculating the spectral density in the general case. Unfortunately, the free multiplicative convolution has no simple expression for matrices of finite size, but in the limit of large size—which is also the limit of a large network—suitable expressions do exist. Specifically, for a spectral density  $\rho$  we can define a function

$$\Gamma_\rho(z) = \int \frac{x \rho(x) dx}{z - x}, \quad (11)$$

which is called the *Cauchy transform* of  $x\rho(x)$ . Then, if  $\rho$  is the free multiplicative convolution of two other distributions  $p$  and  $\rho_c$  as in Eq. (10), it can be shown that

$$\Gamma_\rho^{-1}(u) = \frac{u}{u+1} \Gamma_p^{-1}(u) \Gamma_{\rho_c}^{-1}(u), \quad (12)$$

where  $\Gamma^{-1}$  denotes the functional inverse of  $\Gamma$ , and  $\Gamma_p$  and  $\Gamma_{\rho_c}$  are defined by analogy with (11),

$$\Gamma_p(z) = \int \frac{k p(k) dk}{z - k}, \quad \Gamma_{\rho_c}(z) = \int \frac{x \rho_c(x) dx}{z - x}. \quad (13)$$

Substituting Eq. (8) into the second of these, we have

$$\begin{aligned} \Gamma_{\rho_c}(z) &= \frac{1}{2\pi} \int_{-2/\sqrt{c}}^{2/\sqrt{c}} \frac{x \sqrt{4c - c^2 x^2}}{z - x} dx \\ &= \frac{1}{2} c z (z \pm \sqrt{z^2 - 4/c}) - 1. \end{aligned} \quad (14)$$

The ambiguity in the sign of the square root arises because of a branch cut in the evaluation of the integral, but it can be shown that the final result for the free convolution never depends on the choice of sign [35]. In the present case, we can take either sign and rearrange for  $z$  as a function of  $\Gamma_{\rho_c}$  and we find that the functional inverse is given by

$$\Gamma_{\rho_c}^{-1}(u) = \frac{u + 1}{\sqrt{cu}}. \quad (15)$$

Substituting this expression into (12) we get

$$\Gamma_\rho^{-1}(u) = \sqrt{\frac{u}{c}} \Gamma_p^{-1}(u), \quad (16)$$

and evaluating this equation at the point  $u = \Gamma_\rho(z)$  gives  $z = \sqrt{\Gamma_\rho(z)/c} \Gamma_p^{-1}(\Gamma_\rho(z))$ , which can be rearranged to read

$$\Gamma_\rho(z) = \Gamma_p(z \sqrt{c/\Gamma_\rho(z)}). \quad (17)$$

For convenience, we define  $h(z) = \sqrt{\Gamma_\rho(z)/c}$  and Eq. (17) becomes

$$ch^2(z) = \Gamma_p(z/h(z)) = \int_0^\infty \frac{k p(k) dk}{z/h(z) - k}, \quad (18)$$

or, more simply,

$$h(z) = \frac{1}{c} \int_0^\infty \frac{k p(k) dk}{z - kh(z)}. \quad (19)$$

If we can solve this equation for  $h(z)$ , then the Cauchy transform of  $x\rho(x)$ , Eq. (11), is given by  $\Gamma_\rho(z) = ch^2(z)$ . To recover  $\rho$  itself from the Cauchy transform, we note that for real  $x$  and  $\eta$

$$-\frac{1}{\pi} \text{Im} \frac{1}{x + i\eta} = \frac{\eta/\pi}{x^2 + \eta^2}, \quad (20)$$

which is a Lorentzian of width  $\eta$  and area 1 and hence in the limit as  $\eta \rightarrow 0^+$  becomes equal to a  $\delta$  function,

$$-\frac{1}{\pi} \lim_{\eta \rightarrow 0^+} \text{Im} \frac{1}{x + i\eta} = \delta(x). \quad (21)$$

Thus,

$$\begin{aligned} z\rho(z) &= \int x\rho(x)\delta(z-x) dx, \\ &= -\frac{1}{\pi} \lim_{\eta \rightarrow 0^+} \text{Im} \int \frac{x\rho(x)}{z-x+i\eta} dx, \\ &= -\frac{1}{\pi} \lim_{\eta \rightarrow 0^+} \text{Im} \Gamma_\rho(z+i\eta). \end{aligned} \quad (22)$$

This is the *Stieltjes-Perron inversion formula*. Setting  $\Gamma_\rho(z) = ch^2(z)$  tells us that the spectral density of the configuration model is given by

$$\rho(z) = -\frac{c}{\pi z} \text{Im} h^2(z), \quad (23)$$

where the imaginary part is taken in the limit as  $z$  tends to the real line from above.

Equations (19) and (23) give us a complete recipe for calculating the spectrum of the modularity matrix. We note that equations equivalent to these have been derived in other contexts in the literature on random matrices. See, for example, the results on band matrices in Refs. [36–40].

### A. Example solutions

The solution of Eqs. (19) and (23) relies on our being able to compute the integral in Eq. (19), whose difficulty depends on the particular choice of degree distribution. To give an example where the calculation is straightforward, consider the standard Poisson random graph, for which all vertices have the same expected degree  $c$  and hence  $p(k) = \delta(k-c)$ . Substituting into (19) and solving the resulting quadratic equation gives

$$h(z) = \frac{z - \sqrt{z^2 - 4c}}{2c}, \quad (24)$$

so the spectral density is

$$\rho(z) = \frac{\sqrt{4c - z^2}}{2\pi c}, \quad (25)$$

which recovers the standard semicircle distribution for the random graph.

As a more general example, consider any distribution where the degrees take a set of  $\ell$  discrete values  $d_r$ , as they do for any integer-valued degree distribution of the type commonly considered for network models. Then  $p(k) = \sum_{r=1}^{\ell} p_r \delta(k - d_r)$ , where the coefficients  $p_r$  satisfy  $\sum_r p_r = 1$ . Then, from Eq. (19),

$$h(z) = \frac{\sum_{r=1}^{\ell} p_r d_r / [z - d_r h(z)]}{\sum_{r=1}^{\ell} p_r d_r}, \quad (26)$$

where we have used  $c = \sum_r p_r d_r$ . Thus,  $h(z)$  is the root of a polynomial of degree  $\ell + 1$ . For instance, if there are two discrete values of the expected degree, then

$$h(z) = \frac{1}{p_1 d_1 + p_2 d_2} \left[ \frac{p_1 d_1}{z - d_1 h(z)} + \frac{p_2 d_2}{z - d_2 h(z)} \right], \quad (27)$$

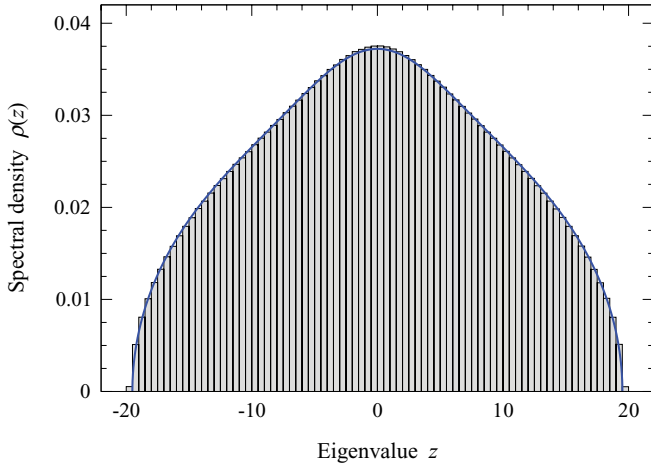


FIG. 1. (Color online) The spectral density  $\rho(z)$  for the degree distribution described in the text, in which vertices have expected degree  $d_1 = 50$  with probability  $p_1 = \frac{1}{4}$  and  $d_2 = 100$  with probability  $p_2 = \frac{3}{4}$ . The curve gives the analytic solution, derived from Eqs. (23) and (28); the histogram shows the results of numerical calculations for actual networks with  $n = 10\,000$  vertices, averaged over 100 different networks.

which can be rearranged to give the cubic equation

$$d_1 d_2 h^3 - (d_1 + d_2) z h^2 + \left[ \frac{d_1 d_2}{p_1 d_1 + p_2 d_2} + z^2 \right] h - z = 0. \quad (28)$$

Of the three solutions to this equation, one is always real, and hence [in light of Eq. (23)] cannot give the spectral density. The remaining two are complex conjugates and so give results that differ only in sign, the positive sign being the one we are looking for.

Figure 1 shows a plot of the resulting spectral density, Eq. (23), as a function of  $z$  for the case  $d_1 = 50$ ,  $d_2 = 100$ , and  $p_1 = 1 - p_2 = \frac{1}{4}$ . The figure shows strong departure from the semicircle law. Also shown are the results of direct numerical calculations of the spectra of simulated networks with the same degree distribution and the agreement between the analytic and numerical results is good.

### B. Features of the spectral density

We can invoke additional properties of the free convolution to better understand the spectrum of the modularity matrix. Consider, for instance, the case where the expected degree distribution  $p(k)$  has compact support, meaning that there are hard upper and lower limits to the expected degree a vertex may have. (The lower limit is trivial, since degrees must be non-negative, but the upper limit is not.) Since the semicircle distribution, Eq. (8), also has compact support, the spectral density of the modularity matrix is then a convolution of two compact distributions. In this scenario it can be shown that the bulk spectrum of the modularity matrix will also have compact support [40]. Furthermore, given this observation, we can show that the spectrum will generically exhibit a sharp square-root decay at its edges. To see this, note that the central function  $h(z)$  in our theory is the solution for  $h$  of an equation of the

form  $f(h, z) = 0$ , where  $z$  is given and

$$f(h, z) = \frac{1}{c} \int_0^\infty \frac{k p(k) dk}{z - kh} - h. \quad (29)$$

[See Eq. (19).] From Eq. (23) we know that  $h$  is complex within the spectral band and real outside it and, hence, the edge of the band is the point at which complex solutions to  $f(h, z) = 0$  disappear. For analytic  $f(h, z)$  such a disappearance corresponds to the point at which an extremum of  $f$  with respect to  $h$  crosses the zero line. Denoting this point by  $(h, z) = (a, b)$  and performing an expansion about it to leading order in both  $h$  and  $z$ , we then have

$$f(h, z) = \frac{\partial f}{\partial z}(z - b) + \frac{\partial^2 f}{\partial h^2}(h - a)^2 + \dots, \quad (30)$$

the terms in  $f(a, b)$  and  $\partial f / \partial h$  vanishing at the extremum. In the limit as we approach the band edge, therefore, the equation  $f(h, z) = 0$  takes the form

$$\frac{\partial f}{\partial z}(z - b) + \frac{\partial^2 f}{\partial h^2}(h - a)^2 = 0, \quad (31)$$

and hence within the band, we have  $h(z) = a + iB\sqrt{b - z}$  for some real constant  $B$ . Then the spectral density, Eq. (23), is

$$\rho(z) = C \frac{\sqrt{b - z}}{z}, \quad (32)$$

where  $C$  is another real constant. A similar argument implies square-root behavior at the lower edge of the spectrum as well. The square-root form can be seen, for example, in the vertical sides of the spectrum in Fig. 1.

We can also calculate the behavior of  $h(z)$  as  $z \rightarrow b$  from above, for which Eq. (31) implies

$$h(z) = a + B\sqrt{z - b}, \quad (33)$$

with the same real constant  $B$  as before. Note that this implies that the limiting value of  $h(z)$  at the band edge is generically finite but that the slope  $dh/dz$  diverges. This has important consequences for “hub” vertices—those with unusually high degree—whose effect on the spectrum displays a phase transition behavior that depends crucially on the functional form of  $h(z)$ . We discuss hub vertices in detail in Sec. VI.

These results apply for the case where the expected degree distribution is bounded. In cases where it is not we expect the spectral density of the modularity matrix to be similarly unbounded, having no band edge and generically inheriting the worst-case tail behavior of  $p(k)$ . Similar observations have been made previously by Chung *et al.* [29] for a different matrix, the graph Laplacian. They note that a normalized version of the Laplacian, akin to our normalized modularity matrix  $\tilde{B}$ , should display a semicircle distribution but that the Laplacian itself should have a spectrum that inherits the tail behavior of the degree distribution.

## IV. THE RESOLVENT AND THE STIELTJES TRANSFORM

In the previous section we calculated the spectral density of the modularity matrix for the configuration model. It is possible to calculate many other properties of the spectrum as well, as we now show. Our starting point for these calculations

is the so-called resolvent matrix, which is the matrix function  $\mathbf{R}(z) = (z\mathbf{I} - \mathbf{B})^{-1}$ , where  $\mathbf{I}$  is the identity. As we will see, a knowledge of the ensemble average of the resolvent allows us to calculate many things, including the spectral density of the adjacency matrix, the leading eigenvalue of the adjacency matrix, and the effect on the spectrum of network hubs.

It also gives us an alternative, though perhaps less elegant, derivation of the results for the modularity matrix in the previous section. The spectral density  $\rho(z)$  of the modularity matrix can be defined as

$$\rho(z) = \frac{1}{n} \sum_{i=1}^n \delta(z - \lambda_i), \quad (34)$$

where  $\lambda_i$  are the eigenvalues of the matrix. Substituting for the  $\delta$  function from Eq. (21), we get the so-called Plemelj-Sokhotski formula,

$$\rho(z) = -\frac{1}{n\pi} \lim_{\eta \rightarrow 0^+} \text{Im} \sum_{i=1}^n \frac{1}{z - \lambda_i + i\eta}. \quad (35)$$

Via a change of basis, the sum on the right-hand side is equal to the trace of the matrix  $[(z + i\eta)\mathbf{I} - \mathbf{B}]^{-1}$ , and hence  $\rho(z)$  is the limit where  $z$  goes to the real line of  $-(1/n\pi)\text{Im} \text{Tr}(z\mathbf{I} - \mathbf{B})^{-1}$ . In other words, the spectral density depends on the trace of the resolvent, and its average over the ensemble of model networks is given by the average of this quantity,

$$\rho(z) = -\frac{1}{n\pi} \text{Im} \text{Tr}(\langle z\mathbf{I} - \mathbf{B} \rangle^{-1}). \quad (36)$$

The normalized trace  $\text{Tr}(z\mathbf{I} - \mathbf{B})^{-1}/n$  is called the *Stieltjes transform* of  $\mathbf{B}$ .

The two most common ways to calculate the Stieltjes transform are either to expand the matrix  $(z\mathbf{I} - \mathbf{B})^{-1}$  in powers of  $\mathbf{B}$  and take the trace term by term or to write the trace in terms of a derivative of a Fresnel integral and then employ the replica trick [41]. Here, however, we take a different approach inspired by work of Bai and Silverstein [16,42] that allows us to calculate the average of the full resolvent.

The resolvent is the inverse of a matrix whose off-diagonal elements are zero-mean random variables. Consider a general such matrix  $\mathbf{X}$  and let us write it in terms of its first  $n-1$  rows and columns, plus the last row and column, thus,

$$\mathbf{X} = \begin{pmatrix} \mathbf{X}_n & \mathbf{a} \\ \mathbf{a}^T & x_{nn} \end{pmatrix}. \quad (37)$$

Thus,  $\mathbf{X}_n$  is the matrix  $\mathbf{X}$  with the  $n$ th row and column removed, and  $\mathbf{a}$  is the  $n$ th column minus its last element  $x_{nn}$ .

Now consider the vector  $\mathbf{v} = \mathbf{X}^{-1}\mathbf{u}$ , where  $\mathbf{u} = (0, \dots, 0, 1)$ . Let us break  $\mathbf{v}$  into its first  $n-1$  elements and its last element  $\mathbf{v} = (\mathbf{v}_1 | v_n)$ , where clearly  $v_n = [\mathbf{X}^{-1}]_{nn}$ . Then we have  $\mathbf{X}\mathbf{v} = \mathbf{u}$  and, hence,

$$\mathbf{X}_n \mathbf{v}_1 + v_n \mathbf{a} = 0, \quad \mathbf{a}^T \mathbf{v}_1 + x_{nn} v_n = 1. \quad (38)$$

The first equation tells us that

$$\mathbf{v}_1 = -v_n \mathbf{X}_n^{-1} \mathbf{a}, \quad (39)$$

and substituting this result into the second gives

$$[\mathbf{X}^{-1}]_{nn} = v_n = \frac{1}{x_{nn} - \mathbf{a}^T \mathbf{X}_n^{-1} \mathbf{a}}. \quad (40)$$

To make further progress, we assume that  $v_n$  is narrowly peaked about its average value in the limit of large system size, meaning its variance about that value vanishes as  $n$  becomes large. We will for the moment take this assumption as given, but it can be justified using results for concentration of measure of random quadratic forms [43], provided vertex degrees are large (so our results, like those of Sec. III, will be exact only for large degrees).

If  $v_n$  is narrowly peaked, then the average of the reciprocal on the right-hand side of (40) is equal to the reciprocal of the average and

$$\langle [\mathbf{X}^{-1}]_{nn} \rangle = \frac{1}{\langle x_{nn} \rangle - \langle \mathbf{a}^T \mathbf{X}_n^{-1} \mathbf{a} \rangle}. \quad (41)$$

Furthermore, if  $v_n$  is narrowly peaked, then the average of Eq. (39) is  $\langle \mathbf{v}_1 \rangle = -v_n \langle \mathbf{X}_n \rangle \langle \mathbf{a} \rangle = 0$  since  $\mathbf{a}$  is independent of  $\mathbf{X}_n$  and  $\langle \mathbf{a} \rangle = 0$ . But the elements of  $\mathbf{v}_1$  are equal to  $[\mathbf{X}^{-1}]_{in}$  and, hence,

$$\langle [\mathbf{X}^{-1}]_{in} \rangle = 0 \quad (42)$$

for  $i \neq n$ . By the same method, we can derive expressions for the inverse of  $\mathbf{X}$  with any row and column removed and hence show that

$$\langle [\mathbf{X}^{-1}]_{ii} \rangle = \frac{1}{\langle x_{ii} \rangle - \langle \mathbf{a}^T \mathbf{X}_i^{-1} \mathbf{a} \rangle} \quad (43)$$

and

$$\langle [\mathbf{X}^{-1}]_{ij} \rangle = 0 \quad \text{for } i \neq j. \quad (44)$$

In other words,  $\langle \mathbf{X}^{-1} \rangle$  is a diagonal matrix when  $n$  is large, with diagonal elements given by Eq. (43).

But if this is true of  $\mathbf{X}^{-1}$ , then by the same argument it must also be true of  $\mathbf{X}_i^{-1}$ . Hence, noting that  $\mathbf{a}$  is independent of  $\mathbf{X}_i$ , we have

$$\langle \mathbf{a}^T \mathbf{X}_i^{-1} \mathbf{a} \rangle = \sum_{jk} \langle [\mathbf{X}_i^{-1}]_{jk} \rangle \langle a_j a_k \rangle = \sum_j \langle [\mathbf{X}_i^{-1}]_{jj} \rangle \langle a_j^2 \rangle. \quad (45)$$

Returning now to Eq. (36), the role of the matrix  $\mathbf{X}$  in our problem is played by  $z\mathbf{I} - \mathbf{B}$ . As we noted earlier, the elements of the modularity matrix  $\mathbf{B}$  (and, hence, also the elements of the vector  $\mathbf{a}$ ) have mean zero and variance  $k_i k_j / 2m$ . Hence,  $\langle a_j^2 \rangle = k_i k_j / 2m$  in Eq. (45) and

$$\begin{aligned} \langle \mathbf{a}^T \mathbf{X}_i^{-1} \mathbf{a} \rangle &= \sum_j \langle [(z\mathbf{I} - \mathbf{B}_i)^{-1}]_{jj} \rangle \frac{k_i k_j}{2m} \\ &= \frac{k_i}{2m} \text{Tr}[\mathbf{D}_i \langle (z\mathbf{I} - \mathbf{B}_i)^{-1} \rangle], \end{aligned} \quad (46)$$

where  $\mathbf{D}$  is the diagonal matrix with elements  $k_i$  as previously and  $\mathbf{D}_i$  is the same matrix with the  $i$ th row and column removed.

However, if  $\text{Tr}[\mathbf{D}_i \langle (z\mathbf{I} - \mathbf{B}_i)^{-1} \rangle] / 2m$  tends to a well-defined limit as the network becomes large, then in this limit it must equal  $\text{Tr}[\mathbf{D} \langle (z\mathbf{I} - \mathbf{B})^{-1} \rangle] / 2m$ —the omission, or not, of the  $i$ th row and column makes a vanishing difference for large  $n$ . Hence, (43) becomes

$$\langle [(z\mathbf{I} - \mathbf{B})^{-1}]_{ii} \rangle = \frac{1}{z - k_i \text{Tr}[\mathbf{D} \langle (z\mathbf{I} - \mathbf{B})^{-1} \rangle] / 2m}, \quad (47)$$

where we have made use of the fact that  $\langle B_{ii} \rangle = 0$ . At the same time, the off-diagonal elements of  $\langle (z\mathbf{I} - \mathbf{B})^{-1} \rangle$  are zero by Eq. (44), so the average of the resolvent matrix is diagonal, a result that will be crucial for several following developments.

Without loss of generality, we now label the vertices of our network in order of increasing expected degree, and for convenience we define functions  $\gamma_z(x)$  and  $k(x)$  of the continuous variable  $x$  thus:

$$\gamma_z(i/n) = \langle [(z\mathbf{I} - \mathbf{B})^{-1}]_{ii} \rangle, \quad k(i/n) = k_i. \quad (48)$$

Then, for large  $n$ , Eq. (47) becomes

$$\gamma_z(x) = \frac{1}{z - [k(x)/c] \int_0^1 k(y) \gamma_z(y) dy}, \quad (49)$$

where  $c = 2m/n$  is the average degree, as previously.

The spectral density, Eq. (36), is related to  $\gamma_z(x)$  by

$$\rho(z) = -\frac{1}{\pi} \text{Im} g(z), \quad (50)$$

where

$$g(z) = \frac{1}{n} \text{Tr} \langle (z\mathbf{I} - \mathbf{B})^{-1} \rangle = \int_0^1 \gamma_z(x) dx, \quad (51)$$

which is just the ensemble average of the Stieltjes transform. To calculate  $g(z)$ , we define the additional quantity

$$\begin{aligned} h(z) &= \frac{1}{2m} \text{Tr}[\mathbf{D} \langle (z\mathbf{I} - \mathbf{B})^{-1} \rangle] = \frac{1}{c} \int_0^1 k(x) \gamma_z(x) dx \\ &= \frac{1}{c} \int_0^1 \frac{k(x) dx}{z - k(x)h(z)}, \end{aligned} \quad (52)$$

where we have used Eq. (49). Since we have labeled our vertices in order of increasing degree,  $k(x)$  is by definition the  $(nx)$ th-lowest degree in the network, or, equivalently, it is the functional inverse of the cumulative distribution function  $P(k)$  defined by

$$P(k) = \int_0^k p(k') dk', \quad (53)$$

where  $p(k)$  is the expected degree distribution. Thus, changing variables from  $x$  to  $k$ , Eq. (52) can be written

$$h(z) = \frac{1}{c} \int_0^\infty \frac{k dP(k)}{z - kh(z)} \quad (54)$$

or as either of the equivalent forms

$$h(z) = \frac{1}{c} \int_0^\infty \frac{k p(k) dk}{z - kh(z)} = \int_0^\infty \frac{q(k) dk}{z - kh(z)}, \quad (55)$$

where the (correctly normalized) probability distribution

$$q(k) = \frac{k p(k)}{c} \quad (56)$$

is known as the *excess degree distribution* in the networks literature. This distribution, which arises often in the theory of networks, is the probability that the network vertex reached by following an edge has an expected number  $k$  of edges attached to it other than the one we followed to reach the vertex. (The distribution looks slightly different from the form usually given [24] because it is expressed in terms of expected degree rather than actual degree.)

If we can solve Eq. (55) for  $h(z)$ , then we can calculate  $g(z)$  by substituting Eq. (49) into Eq. (51) and again changing variables from  $x$  to  $k$  to get

$$g(z) = \int_0^\infty \frac{p(k) dk}{z - kh(z)}. \quad (57)$$

This equation is similar in form to Eq. (55), but note that it is the ordinary degree distribution  $p(k)$  that appears in the numerator, not the excess degree distribution.

Alternatively, and more directly, we can calculate  $g(z)$  by multiplying both sides of (49) by the right-hand denominator, integrating, and rearranging to get

$$g(z) = \frac{1 + ch^2(z)}{z}. \quad (58)$$

Combining this result with Eq. (50) now gives us the spectral density

$$\rho(z) = -\frac{c}{\pi z} \text{Im} h^2(z), \quad (59)$$

where the imaginary part is, if necessary, calculated as the limit where  $z$  tends to the real line from above.

Equations (55) and (59) are precisely the equations (19) and (23) that we derived previously using the free convolution.

## V. SPECTRUM OF THE ADJACENCY MATRIX

In the previous sections we have derived the spectral density of the modularity matrix. To calculate the corresponding quantity for the adjacency matrix we make use of an argument of [44,45] as follows. The adjacency matrix can be written in terms of the modularity matrix as  $\mathbf{A} = \mathbf{B} + \mathbf{k}\mathbf{k}^T / 2m$ , where  $\mathbf{k}$  is the  $n$ -element vector with elements  $k_i$ . Hence any eigenvalue-vector pair  $z, \mathbf{v}$  of the adjacency matrix satisfies

$$\left( \mathbf{B} + \frac{\mathbf{k}\mathbf{k}^T}{2m} \right) \mathbf{v} = z\mathbf{v}, \quad (60)$$

which can be rearranged to read

$$\frac{\mathbf{k}^T \mathbf{v}}{2m} (z\mathbf{I} - \mathbf{B})^{-1} \mathbf{k} = \mathbf{v}. \quad (61)$$

Multiplying by  $\mathbf{k}^T$ , we then find that

$$\frac{1}{2m} \mathbf{k}^T (z\mathbf{I} - \mathbf{B})^{-1} \mathbf{k} = 1. \quad (62)$$

Expanding  $\mathbf{k}$  as a linear combination of the eigenvectors  $\mathbf{b}_i$  of  $\mathbf{B}$ , this result can be written

$$\frac{1}{2m} \sum_{i=1}^n \frac{(\mathbf{k}^T \mathbf{b}_i)^2}{z - \beta_i} = 1, \quad (63)$$

where  $\beta_i$  are the eigenvalues of the modularity matrix.

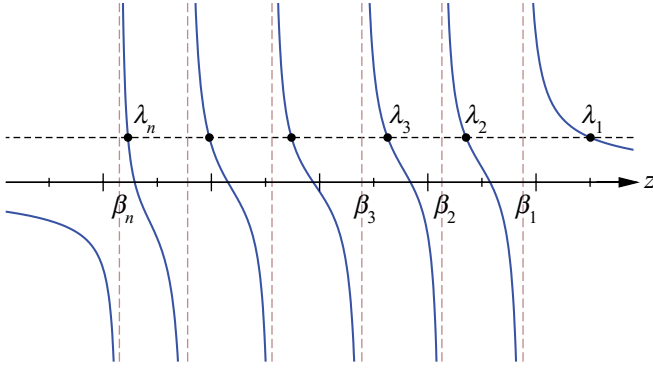


FIG. 2. (Color online) The solutions  $\lambda_i$  to Eq. (63) correspond to the points where the left-hand side of the equation (solid curves) equals 1 (dashed horizontal line). This implies that the values of the  $\lambda_i$  are interleaved between the eigenvalues  $\beta_i$  of the modularity matrix.

The solutions of this equation can be visualized as in Fig. 2. The solid curves represent the left-hand side of the equation, which has poles as shown at  $z = \beta_i$  for all  $i$ . The dashed horizontal line represents the 1 on the right-hand side and the points at which it intercepts the curves are the solutions for  $z$  of (63), which are the eigenvalues  $\lambda_i$  of the adjacency matrix. If we number the eigenvalues of both  $\mathbf{A}$  and  $\mathbf{B}$  in order from largest to smallest, the geometry of Fig. 2 implies that the eigenvalues must satisfy an interleaving condition of the form  $\lambda_1 \geq \beta_1 \geq \lambda_2 \geq \beta_2 \geq \dots \geq \lambda_n \geq \beta_n$ . In the limit of large  $n$ , where the spectral density of the modularity matrix becomes a smooth function and the eigenvalues are arbitrarily closely spaced, this implies that  $\lambda_i \rightarrow \beta_i$ , so asymptotically the spectral density of the adjacency matrix is the same as that of the modularity matrix.

The only exception is the highest eigenvalue of the adjacency matrix  $\lambda_1$ , which is bounded below by  $\beta_1$ , but unbounded above. To calculate this value we average (62) over the ensemble and recall, as demonstrated in Sec. IV, that  $\langle (z\mathbf{I} - \mathbf{B})^{-1} \rangle$  is diagonal and, hence,

$$\frac{1}{2m} \mathbf{k}^T \langle (z\mathbf{I} - \mathbf{B})^{-1} \rangle \mathbf{k} = \frac{1}{2m} \sum_i k_i^2 \langle [(z\mathbf{I} - \mathbf{B})^{-1}]_{ii} \rangle. \quad (64)$$

Combining this result with (62) and using Eq. (48), we then have

$$\frac{1}{c} \int_0^1 k^2(x) \gamma_z(x) dx = 1. \quad (65)$$

Taking Eq. (49), multiplying by the right-hand denominator and a further factor of  $k(x)$ , and then integrating over  $x$ , we get

$$czh(z) - h(z) \int_0^1 k^2(x) \gamma_z(x) dx = \int_0^1 k(x) dx. \quad (66)$$

And combining this result with Eq. (65) and noting that  $\int_0^1 k(x) dx = \int_0^\infty k p(k) dk = c$ , we have

$$(z - 1)h(z) = 1. \quad (67)$$

The solution of this equation for  $z$  gives us the leading eigenvalue  $\lambda_1$  of the adjacency matrix.

For the Poisson random graph, for example, this result, in combination with Eq. (24), tells us that the leading eigenvalue

takes the value  $c + 1$ . This is not a new result—it is well known in the literature—but it is comforting to see that the formalism works.

For the two-degree model of Eq. (27), we can use (67) to eliminate  $h(z)$  from (27) and get

$$\frac{p_1 d_1 + p_2 d_2}{(z - 1)^2} = \frac{p_1 d_1}{z(z - 1) - d_1} + \frac{p_2 d_2}{z(z - 1) - d_2}, \quad (68)$$

which gives us a cubic equation for  $z$ . For the parameter values used in Fig. 1, for example,  $d_1 = 50$ ,  $d_2 = 100$ , and  $p_1 = 1 - p_2 = \frac{1}{4}$ , we find that the leading eigenvalue of the adjacency matrix is  $z = 93.893 \dots$ . A numerical calculation for the same parameters is in good agreement, giving  $z = 93.896 \pm 0.017$  for an average over 100 systems of size  $n = 10000$ .

For the case of general degree distribution, we can use (67) to eliminate  $h(z)$  in Eq. (55) to get

$$\frac{z}{z - 1} = \int_0^\infty \frac{q(k) dk}{1 - k/(z^2 - z)}. \quad (69)$$

An exact solution to this equation requires us to perform the integral, but one can derive an approximate solution by expanding the denominator of the integrand,

$$\frac{z}{z - 1} = 1 + \int_0^\infty \sum_{r=1}^{\infty} \frac{k^r}{(z^2 - z)^r} q(k) dk \quad (70)$$

or

$$\frac{1}{z - 1} = \sum_{r=1}^{\infty} \frac{\langle k^r \rangle_q}{(z^2 - z)^r}, \quad (71)$$

where  $\langle \dots \rangle_q$  denotes an average over the excess degree distribution of Eq. (56). If  $z^2 - z \gg k_{\max}$ , where  $k_{\max}$  is the largest degree in the network, and noting that  $\langle k^r \rangle_q \leq k_{\max}^r$ , we have

$$\frac{1}{z - 1} = \frac{\langle k \rangle_q}{z^2 - z} + O[k_{\max}/(z^2 - z)]^2 \quad (72)$$

or

$$z \simeq \frac{\langle k^2 \rangle}{\langle k \rangle} \quad (73)$$

to leading order, where we have made use of  $\langle k \rangle_q = \langle k^2 \rangle / \langle k \rangle$ . This result was derived previously by other means by Chung *et al.* [29].

Taking the example of the two degree model above again, this approximation gives

$$z \simeq \frac{p_1 d_1^2 + p_2 d_2^2}{p_1 d_1 + p_2 d_2}, \quad (74)$$

and for the parameter values of Fig. 1 we find that  $z \simeq 92.86$ , which differs by about 1% from the true value of 93.89 given by Eq. (68).

## VI. NETWORK HUBS

The picture developed in the previous sections is one in which the spectrum of the adjacency matrix has two primary components: a single leading eigenvalue plus a continuous band of lower eigenvalues, which it shares with the modularity matrix.



Let us examine more closely the continuous band and concentrate on the case of the modularity matrix, which is simpler since it has only the band and no separate leading eigenvalue. Consider the eigenvalues that lie at the topmost edge of the band, which are the highest eigenvalues of the modularity matrix. These eigenvalues are normally associated with good bisections of the network into “communities”—if a good bisection exists, then there will be a corresponding high-lying eigenvalue whose eigenvector’s elements describe the split [6].

As we now argue, however, there is another mechanism that generates high-lying eigenvalues, namely the presence of hubs in the network—vertices of unusually high degree—and the highest eigenvalues in the spectrum of the modularity matrix, and also the lowest, are often due to these hubs, while those corresponding to communities are somewhat smaller. As we will see, for hubs of sufficiently high degree, these eigenvalues can split off from the continuous band in a manner reminiscent of impurity states in condensed matter physics. In effect, the hub acts as an impurity in the network.

To see how the addition of a hub to a network produces a high-lying eigenvalue, let the hub be vertex  $n$  and let  $\mathbf{B}_n$  once again be the modularity matrix without the  $n$ th vertex (i.e., with the  $n$ th row and column removed), so the full modularity matrix looks like this:

$$\mathbf{B} = \begin{pmatrix} \mathbf{B}_n & \mathbf{a} \\ \mathbf{a}^T & b_{nn} \end{pmatrix}. \quad (75)$$

Now, in an argument analogous to that of the previous section, consider an eigenvector of this matrix  $\mathbf{v} = (\mathbf{v}_1|v_n)$ . Then the eigenvector equation  $\mathbf{B}\mathbf{v} = z\mathbf{v}$  can be multiplied out to give the equations

$$\mathbf{B}_n\mathbf{v}_1 + v_n\mathbf{a} = z\mathbf{v}_1, \quad (76)$$

$$\mathbf{a}^T\mathbf{v}_1 + b_{nn}v_n = zv_n. \quad (77)$$

The first of these can be rearranged to give

$$\mathbf{v}_1 = v_n(z\mathbf{I} - \mathbf{B}_n)^{-1}\mathbf{a}. \quad (78)$$

Multiplying by  $\mathbf{a}^T$  and using the second equation then gives

$$\mathbf{a}^T(z\mathbf{I} - \mathbf{B}_n)^{-1}\mathbf{a} = z - b_{nn}. \quad (79)$$

Now we note that the  $i$ th element of  $\mathbf{a}$  is an independent random variable with variance  $k_n k_i / 2m$  and we can average over the ensemble and apply Eq. (45) to rewrite the left-hand side, giving

$$\frac{k_n}{2m} \text{Tr}[\mathbf{D}_n \langle (z\mathbf{I} - \mathbf{B}_n)^{-1} \rangle] = z, \quad (80)$$

where  $\mathbf{D}$  is the diagonal matrix with elements  $k_i$  as before,  $\mathbf{D}_n$  is the same matrix with the  $n$ th row and column removed, and we have made use of the fact that  $\langle b_{nn} \rangle = 0$ . We note, as previously, that if the quantity  $\text{Tr}[\mathbf{D}_n \langle (z\mathbf{I} - \mathbf{B}_n)^{-1} \rangle] / 2m$  tends to a limit as the network becomes large, then that limit is equal to the function  $h(z)$  defined in Eq. (52). Thus, the eigenvalue

$z$  satisfies

$$h(z) = \frac{z}{k_n}. \quad (81)$$

Substituting this expression into Eq. (55) and rearranging, we get an explicit expression for the eigenvalue:

$$z^2 = \frac{k_n^2}{c} \int_0^\infty \frac{k p(k) dk}{k_n - k}. \quad (82)$$

This calculation also extends to the case where there is more than one hub in the network. Because the hub is treated no differently from any other network vertex, the same arguments apply if we add a second hub, or more, after the first. Equation (82) will give the correct eigenvalue for each hub separately.

Once again, our ability to actually solve for the value of  $z$  will depend on whether we can do the integral in Eq. (82) (although one could also evaluate the integral numerically). In the special case where the hub degree  $k_n$  is much larger than the expected degree of any of the other vertices, so that  $k_n - k \simeq k_n$  in the denominator of the integrand, the expression simplifies to

$$z^2 = \frac{k_n}{c} \int_0^\infty k p(k) dk = k_n, \quad (83)$$

and, hence,  $z = \sqrt{k_n}$ .

The solutions of Eq. (81) can be represented graphically as in Fig. 3. The curves in the figure represent the function  $h(z)$  and the diagonal lines represent  $z/k_n$ . The point where the two cross give the eigenvalues. As the figure shows, when the expected degree  $k_n$  of the  $n$ th vertex is large enough, the equation has two solutions, one for low  $z$  and one for high and both given by Eq. (82), that are separate from the continuous spectrum of eigenvalues we calculated in Sec. III.

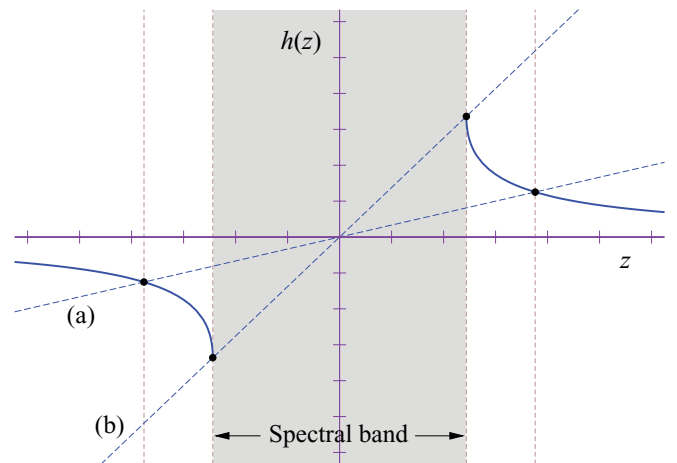


FIG. 3. (Color online) Graphical solution of Eq. (81). The solid curves represent the value of  $h(z)$  as a function of  $z$ , above and below the spectral band, and the hub eigenvalues, which are solutions of Eq. (81), fall at the points where this curve intersects the straight line  $z/k_n$ , represented by the dashed diagonal line. The slope of this line is  $1/k_n$ , and hence when  $k_n$  is large enough, the lines intersect—case (a)—and we have two hub eigenvalues, one above and one below the band (marked by dots). Case (b) is the borderline case. If  $k_n$  is any less than this value, then there is no intersection and the highest and lowest eigenvalues will be those at the band edges.

How high a degree does a hub have to have to generate eigenvalues of this kind? The answer can be seen from Fig. 3— $k_n$  must be large enough for the line  $z/k_n$  to intercept the curve of  $h(z)$ . Thus, there is a critical value of  $k_n$ , represented by the steeper diagonal in the figure, below which the hub eigenvalues vanish. Below this point, the highest eigenvalue will fall at the edge of the continuous band as normal and there will be no special hub eigenvalue. We can derive an expression for the transition point by observing that, as shown in Sec. III B, the slope of  $h(z)$  diverges at the band edge, which implies that  $dz/dk_n = 0$ . Differentiating Eq. (82) and setting the result to zero, we find that the critical value of  $k_n$  is the solution of

$$\int_0^\infty \frac{k p(k) dk}{k_n - k} = \int_0^\infty \frac{k^2 p(k) dk}{(k_n - k)^2}. \quad (84)$$

For example, in the case of the Poisson random graph, this implies that the transition takes place at the point where  $c/(k_n - c) = c^2/(k_n - c)^2$ , i.e., when  $k_n = 2c$ . Thus, we must have  $k_n > 2c$  for the hub to have an effect on the spectrum.

This gives us a working definition of what we mean by a “hub” in a network. It depends, not surprisingly, on the degree distribution of the rest of the network—what it takes to stand out in a crowd depends on the rest of the crowd. But in the Poisson random graph, for instance, a hub is a hub, in spectral terms, if its degree is greater than twice the average in the rest of the network. This is an unexpected result, given that vertices of high degree are easily spotted long before this point is reached, at least for large  $c$ . Since the standard deviation of the degree distribution is  $\sqrt{c}$ , a vertex with degree twice the mean is  $\sqrt{c}$  standard deviations above the mean, which is a large number for large  $c$ .

Nonetheless, the result does appear to be correct. Figure 4 shows the results of numerical calculations of the largest eigenvalue of the modularity matrix for a Poisson random graph with a single additional hub of expected degree  $k_n$ , as a function of  $k_n$ . As the figure shows, the eigenvalue obeys Eq. (82) quite closely until  $k_n$  falls below  $2c$  (the vertical dashed line). Past this point, the leading eigenvalue assumes the same value  $2\sqrt{c}$  as in a standard Poisson random graph with no hub (the horizontal line), even though the hub may still be present.

Outlying eigenvalues reminiscent of those generated by hub vertices have also been observed in other circumstances. For instance, in networks with modular structure, where vertices break into tightly connected groups with only sparse intergroup connections, eigenvectors are observed outside the continuous spectral band when communities are sufficiently strong [46–49]. The mechanism by which these eigenvalues are generated, however, is distinct from the hub-based mechanism discussed in this section.

Putting together our principal observations, we have now developed quite a complete picture of the spectrum of the configuration model. We expect the spectrum to have two main parts plus a third when the degree distribution implies the presence of hubs:

(1) There is a single eigenvalue given by the solution of Eq. (67), which will normally be the leading eigenvalue.

(2) There is a continuous band, given by Eq. (23). For bounded degree distributions the band will also be bounded,

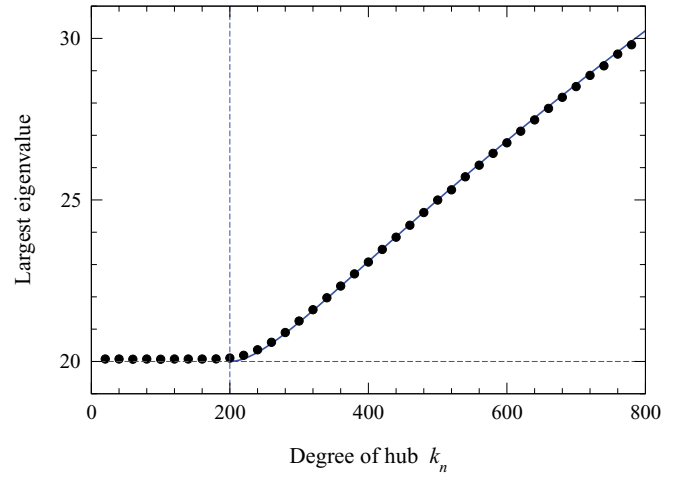


FIG. 4. (Color online) The largest eigenvalue of the modularity matrix for a Poisson random graph of mean degree  $c = 100$  plus a single additional hub of expected degree  $k_n$ . Points are numerical results, averaged over 1000 networks of  $n = 10000$  vertices each. Statistical errors on the measurements are smaller than the points in all cases. The solid curve is Eq. (82), which gives  $z = k_n/\sqrt{k_n - c}$  in this case, and the horizontal dashed line represents the value  $z = 2\sqrt{c} = 20$ , which is the lower limit on the eigenvalue set by the edge of the continuous spectral band. The vertical dashed line represents the critical value  $k_n = 200$  of the hub degree, set by Eq. (84).

both above and below, and have edges that decay to zero as a square root.

(3) If there are hubs in the network, then there will be additional eigenvalues outside the band at both ends, given by Eq. (82). Each hub contributes two eigenvalues, one at each end of the band.

#### A. Localization around hubs

One can also look at the eigenvector corresponding to a hub eigenvalue, which turns out to be heavily localized around the hub vertex. All the elements of the eigenvector, except for the element  $v_n$  corresponding to the hub itself, are given in terms of  $v_n$  by Eq. (78). For given  $\mathbf{a}$ , the expected value of the  $i$ th component is

$$v_i = v_n \langle (\mathbf{z}\mathbf{I} - \mathbf{B}_n)^{-1} \mathbf{a} \rangle_i = v_n \langle (\mathbf{z}\mathbf{I} - \mathbf{B}_n)^{-1} \rangle_{ii} a_i, \quad (85)$$

where we have once again made use of the fact that  $\langle (\mathbf{z}\mathbf{I} - \mathbf{B}_n)^{-1} \rangle$  is diagonal [see Eq. (44)].

The  $i$ th element of the vector  $\mathbf{a}$  takes the value  $a_i = 1 - k_i k_n / 2m$  for vertices  $i$  that are connected to the hub and  $-k_i k_n / 2m$  for those that are not. Hence, in the limit of large  $n$ , eigenvector elements corresponding to neighbors of the hub will be of order a constant, with expected value

$$v_i = v_n \gamma_z(i/n) = \frac{v_n}{z - k_i h(z)} = \frac{v_n}{z(1 - k_i/k_n)}, \quad (86)$$

with  $z$  given by Eq. (82), while the remaining elements will be of order  $1/n$ .

The value of  $v_n$  can be determined by insisting that the complete eigenvector be normalized. Using Eq. (78) we can

write the normalization condition in the form

$$\begin{aligned} 1 &= |\mathbf{v}|^2 = v_n^2 + |\mathbf{v}_1|^2 = v_n^2 [1 + \mathbf{a}^T (z\mathbf{I} - \mathbf{B})^{-2} \mathbf{a}] \\ &= v_n^2 \left[ 1 - \frac{d}{dz} \mathbf{a}^T (z\mathbf{I} - \mathbf{B})^{-1} \mathbf{a} \right]. \end{aligned} \quad (87)$$

When we average over the ensemble we have, by analogy with Eq. (46),

$$\langle \mathbf{a}^T (z\mathbf{I} - \mathbf{B})^{-1} \mathbf{a} \rangle = \frac{k_n}{2m} \text{Tr}(\mathbf{D}(z\mathbf{I} - \mathbf{B})^{-1}) = k_n h(z), \quad (88)$$

and, hence, (87) implies that

$$v_n^2 = \frac{1}{1 - k_n h'(z)}, \quad (89)$$

where  $h'(z)$  denotes the first derivative of  $h(z)$ , and we are assuming once again that the vector element  $v_n$  is narrowly peaked about its expected value. Note that  $h'(z)$  is negative at both the positive and negative band edges and diverges to  $-\infty$  as we approach the band edge. Thus  $v_n \rightarrow 0$  as we approach the transition at the which the hub eigenvalue disappears.

The results above apply to the hub eigenvectors at both ends of the spectral band, there being two eigenvalues for each hub vertex, one at either end, as shown in the previous section. Both eigenvectors will have a single element of order 1 in the position corresponding to the hub itself, elements of order  $1/z$  in the positions corresponding the neighbors of the hub [see Eq. (86)], and all other elements of order  $1/n$ . In other words, both eigenvectors are strongly localized in the neighborhood of the hub. The only qualitative difference between the two eigenvectors is in the sign of the elements corresponding to the neighbors which, because of Eq. (86), will have the same sign as  $v_n$  for the positive eigenvalue and the opposite sign for the negative one. Localization around hubs has been observed numerically in the past for a different class of network models,

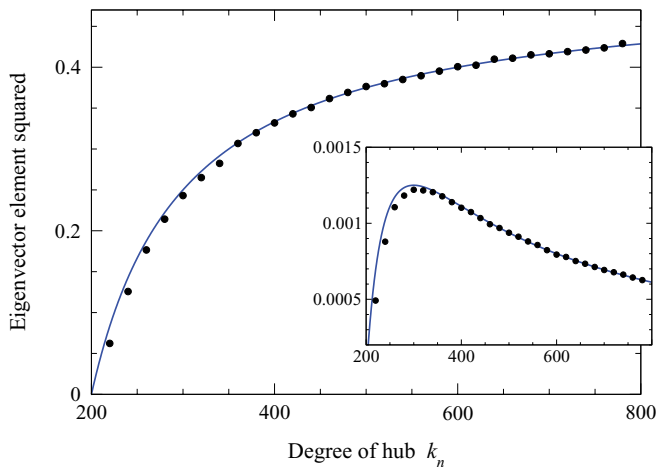


FIG. 5. (Color online) Values of elements of the leading eigenvector of the modularity matrix for a Poisson random graph with  $n = 10\,000$  vertices and mean degree  $c = 100$ , with a single added hub of degree  $k_n$ . Main figure: value of the vector element corresponding to the hub itself. Inset: average value of the elements corresponding to the hub's immediate network neighbors. Points are numerical results, averaged over 100 networks each; curves are the analytic prediction, Eq. (90). Statistical errors are smaller than the data points in all cases.

the preferential attachment models, by Goh *et al.* [50], but has not to our knowledge been demonstrated analytically or studied in the configuration model.

As an example of the above results, consider again the Poisson random graph, for which  $h(z)$  is given by Eq. (24) and  $z$  is given by Eq. (82) to be  $\pm k_n / \sqrt{k_n - c}$ , so  $h'(z) = -1/(k_n - 2c)$  and the expected values of the eigenvector elements at both ends of the spectrum satisfy

$$v_i^2 = \begin{cases} (\frac{1}{2}k_n - c)/(k_n - c) & \text{for } i = n, \\ (\frac{1}{2}k_n - c)/(k_n - c)^2 & \text{for } i \text{ a neighbor of } n, \\ 0 & \text{otherwise,} \end{cases} \quad (90)$$

in the limit of large network size. Figure 5 shows a comparison of these predictions with numerical results for actual networks. As the figure shows, the agreement is once again good, although, as with some of the other calculations, there are small disparities close to the transition at which the hub eigenvalue meets the band edge (which is at  $k_n = 200$  in this case).

## VII. CONCLUSIONS

In this paper we have studied the spectra of the adjacency and modularity matrices of random networks with given expected degrees. Our principal findings are that the spectral densities of the adjacency and modularity matrices are the same in the limit of large system size, except that the adjacency matrix has an additional highest eigenvalue and that the spectral densities are given by the free multiplicative convolution of the degree distribution with a Wigner semicircle distribution. We have confirmed these results with numerical studies of actual networks generated according to the model. The spectra show strong departures from the classical semicircle law, in agreement with numerical studies by previous authors.

We have also studied the effect of network hubs, vertices of unusually high degree, and find that when their degree is sufficiently large these give rise to eigenvalues outside the main band of the spectrum, akin to impurity states in condensed matter systems. We have derived an explicit formula for these hub eigenvalues and we show that the corresponding eigenvectors are strongly localized around the hubs themselves.

In addition to their relevance to partitioning, community structure, and dynamical systems on networks, the techniques developed here could form a starting point for spectral calculations in more elaborate networks. There has, for instance, been recent interest in the spectral properties of community structured networks [46,49], but calculations have been limited to models with Poisson degree distribution. Applications of the methods presented here to such networks could lead to new results for structured networks with nontrivial degree distributions.

## ACKNOWLEDGMENTS

The authors thank Lenka Zdeborova for useful conversations. This work was funded in part by the National Science Foundation under Grants No. CCF-1116115 and No. DMS-1107796 and by the Army Research Office under MURI Grant No. W911NF-11-1-0391.

- [1] M. E. J. Newman, *SIAM Rev.* **45**, 167 (2003).
- [2] S. Boccaletti, V. Latora, Y. Moreno, M. Chavez, and D.-U. Hwang, *Phys. Rep.* **424**, 175 (2006).
- [3] M. Fiedler, *Czech. Math. J.* **23**, 298 (1973).
- [4] A. Pothen, H. Simon, and K.-P. Liou, *SIAM J. Matrix Anal. Appl.* **11**, 430 (1990).
- [5] B. Bollobás, C. Borgs, J. Chayes, and O. Riordan, *Ann. Probab.* **38**, 150 (2010).
- [6] M. E. J. Newman, *Proc. Natl. Acad. Sci. USA* **103**, 8577 (2006).
- [7] S. Fortunato, *Phys. Rep.* **486**, 75 (2010).
- [8] A. Arenas, A. Díaz-Guilera, J. Kurths, Y. Moreno, and C. Zhou, *Phys. Rep.* **469**, 93 (2008).
- [9] A. Barrat, M. Barthélemy, and A. Vespignani, *Dynamical Processes on Complex Networks* (Cambridge University Press, Cambridge, 2008).
- [10] I. J. Farkas, I. Derényi, A.-L. Barabási, and T. Vicsek, *Phys. Rev. E* **64**, 026704 (2001).
- [11] R. Solomonoff and A. Rapoport, *Bull. Math. Biophys.* **13**, 107 (1951).
- [12] P. Erdős and A. Rényi, *Publ. Math. Inst. Hung. Acad. Sci.* **5**, 17 (1960).
- [13] L. Arnold, *Probab. Theory Relat. Fields* **19**, 191 (1971).
- [14] Z. Füredi and J. Komlós, *Combinatorica* **1**, 233 (1981).
- [15] G. Anderson, A. Guionnet, and O. Zeitouni, *An Introduction to Random Matrices* (Cambridge University Press, Cambridge, 2010).
- [16] Z. Bai and J. Silverstein, *Spectral Analysis of Large Dimensional Random Matrices* (Springer-Verlag, Berlin, 2010).
- [17] P. van Mieghem, *Graph Spectra for Complex Networks* (Cambridge University Press, Cambridge, 2011).
- [18] L. Erdos, A. Knowles, H. Yau, and J. Yin, arXiv:1103.1919 (2011).
- [19] T. Tao, *Topics in Random Matrix Theory* (American Mathematical Society, Providence, RI, 2012).
- [20] T. Tao and V. Vu, arXiv:1202.0068 (2012).
- [21] B. Bollobás, *Eur. J. Combinatorics* **1**, 311 (1980).
- [22] M. Molloy and B. Reed, *Random Struct. Algor.* **6**, 161 (1995).
- [23] M. Molloy and B. Reed, *Comb. Prob. Comput.* **7**, 295 (1998).
- [24] M. E. J. Newman, S. H. Strogatz, and D. J. Watts, *Phys. Rev. E* **64**, 026118 (2001).
- [25] R. Cohen, K. Erez, D. ben-Avraham, and S. Havlin, *Phys. Rev. Lett.* **85**, 4626 (2000).
- [26] D. S. Callaway, M. E. J. Newman, S. H. Strogatz, and D. J. Watts, *Phys. Rev. Lett.* **85**, 5468 (2000).
- [27] S. N. Dorogovtsev, A. V. Goltsev, J. F. F. Mendes, and A. N. Samukhin, *Phys. Rev. E* **68**, 046109 (2003).
- [28] R. Kühn, *J. Phys. A* **41**, 295002 (2008).
- [29] F. Chung, L. Lu, and V. Vu, *Proc. Natl. Acad. Sci. USA* **100**, 6313 (2003).
- [30] F. Chung and L. Lu, *Proc. Natl. Acad. Sci. USA* **99**, 15879 (2002).
- [31] D. Voiculescu, K. Dykema, and A. Nica, *Free Random Variables*, Vol. 1 (American Mathematical Society, Providence, RI, 1992).
- [32] G. J. Rodgers and A. J. Bray, *Phys. Rev. B* **37**, 3557 (1988).
- [33] N. Rao and A. Edelman, *Found. Comput. Math.* **8**, 649 (2008).
- [34] S. Olver and R. Nadakuditi, arXiv:1203.1958 (2012).
- [35] N. Rao and R. Speicher, *Electron. Commun. Probab.* **12**, 248 (2007).
- [36] S. Molchanov, L. Pastur, and A. Khorunzhii, *Theor. Math. Phys.* **90**, 108 (1992).
- [37] D. Shlyakhtenko, *Int. Math. Res. Notices* **1996**, 1013 (1996).
- [38] G. Anderson and O. Zeitouni, *Probab. Theory Relat. Fields* **134**, 283 (2006).
- [39] G. Casati and V. Girko, *Random Operators and Stochastic Equations* **1**, 15 (1993).
- [40] Z. Bai and L. Zhang, *J. Multivariate Anal.* **101**, 1927 (2010).
- [41] S. F. Edwards and R. C. Jones, *J. Phys. A* **9**, 1595 (1976).
- [42] Z. Bai, *Statist. Sinica* **9**, 611 (1999).
- [43] N. El Karoui and H. Koesters, arXiv:1105.1404 (2011).
- [44] M. Capitaine, C. Donati-Martin, and D. Féral, *Ann. Probab.* **37**, 1 (2009).
- [45] F. Benaych-Georges and R. R. Nadakuditi, *Adv. Math.* **227**, 494 (2011).
- [46] S. Chauhan, M. Girvan, and E. Ott, *Phys. Rev. E* **80**, 056114 (2009).
- [47] B. Georgeot, O. Giraud, and D. L. Shepelyansky, *Phys. Rev. E* **81**, 056109 (2010).
- [48] S. Jalan, G. Zhu, and B. Li, *Phys. Rev. E* **84**, 046107 (2011).
- [49] R. R. Nadakuditi and M. E. J. Newman, *Phys. Rev. Lett.* **108**, 188701 (2012).
- [50] K.-I. Goh, B. Kahng, and D. Kim, *Phys. Rev. E* **64**, 051903 (2001).