Fracton density of states by the maximum-entropy method

S. N. Evangelou
Physics Department, University of Ioannina, P. O. Box 1186 GR-451 10, Ioannina, Greece and Research Center of Crete, Foundation for Research and Technology (FO.R.TH.), Institute for Electronic Structure and Lasers, Heraklion, P. O. Box 1527, Crete, Greece

N. I. Papanicolaou
Physics Department, University of Ioannina, P. O. Box 1186 GR-451 10, Ioannina, Greece

E. N. Economou
Research Center of Crete, Foundation for Research and Technology (FO.R.TH.), Institute for Electronic Structure and Lasers, Heraklion, P. O. Box 1527 Crete, Greece

(Received 9 August 1990)

We present a study of the one-magnon density of states in the three-dimensional dilute Heisenberg ferromagnet. The ensemble-averaged density of states is evaluted by calculating a small number of spectral moments and employing a maximum-entropy criterion. Finite-size-lattice data, via common numerical simulation techniques, are also presented. The results demonstrate the fracton excitations at the percolation concentration p_c as expected from the Alexander-Orbach conjecture and show the presence of the magnon-to-fracton crossover. At the percolation threshold p_c, we estimate a value for the spectral dimension of $d_s \approx 1.52$. The corresponding problem of phonons in random materials is also discussed in connection with the available experimental data.

I. INTRODUCTION

There is intensive current interest in the study of spin-wave excitations in randomly dilute ferromagnets. Within the Anderson theory of localization it is expected that dilution, which is a geometrical kind of disorder,[1] will drastically affect the spectral and transport properties of one-magnon excitations in a way similar to what disorder does to electrons in metals. In the usual picture of Anderson localization, mobility edges may appear in the energy spectrum that separate extended states, having amplitude constant on average, from localized states that usually decay exponentially. Very rich localization properties are also expected for spin waves in dilute magnets. Classical localization of excitations on finite clusters of connected sites may occur but strong localization for special energies is also common even on the infinite percolating cluster due to its self-similar fractal geometry. The problem can be treated at the percolation threshold where the percolation correlation length diverges and the underlying lattice is known to be a random fractal object on all length scales. The solutions of the Schrödinger equation in this limit are well understood.[2] The excitations are named fractons and the asymptotic behavior of the density of states is reasonably well known. In this paper we investigate the spectral properties of magnon excitations on site-dilute three-dimensional lattices. Our results are also relevant for phonons or classical diffusion. In particular, we considered the spectral density of states for any given amount of dilution by combining the results of an exact calculation of spectral moments with a maximum-entropy method. Our first aim is to point out that the method of moments when combined with the maximum-entropy technique allows a reasonable semi-analytical treatment of spectral density problems in high-dimensional disordered lattices. As an alternative we also present a computational study of the spin-wave density of states. We set up and diagonalize a Hamiltonian matrix ensemble as a function of the concentration p in three dimensions. Such accurate methods, as the exact diagonalization Monte Carlo technique become exceedingly difficult in this case due to the large coordination number of the lattice. The two techniques we use are shown to be powerful and largely complementary. In particular, the usefulness of the moments maximum-entropy method is exploited in comparison with the more accurate numerical data and other approximate effective medium approaches. However, our main purpose is to clarify certain questions concerning the fracton states in three dimensions, such as the estimation of the spectral fracton dimension and the study of the magnon-fracton crossover.

The problem of calculating the magnon density of states in high-dimensional disordered lattices is usually dealt with self-consistent-type mean-field theories, such as the coherent-potential approximation (CPA).[3,4] Although the CPA is the best approximate method known to treat disorder and is widely applicable in dilute systems or alloys it cannot be easily improved. Recently, it was shown[5] that the maximum-entropy method can be an alternative approach to the reconstruction of a spectral density if a small number of its spectral moments are exactly known. Maximum-entropy methods for the solution of undetermined inverse problems have been introduced a long time ago.[6] They are useful approximations when there is a limited supply of data since they are max-

imally noncommittal with respect to missing information. The method for determining densities of states was mathematically founded in Ref. 5 and subsequently applied to various physical problems including various kinds of disordered systems (see, e.g., Ref. 7). It proceeds as follows. The density of states is written as the exponential of a polynomial whose coefficients are subsequently self-consistently determined. The advantage of the technique is that even a small number of given moments for an unknown spectral density is sufficient in order to recover its basic features. The details of the method and its numerical implementation can be found in Ref. 5. Our purpose is the application of this powerful technique to the problem of one-magnon density of states in dilute magnets, including the fracton density of excitations at the percolation threshold.

II. THE MODEL

We consider the one-magnon dynamical matrix equation arising from the Heisenberg Hamiltonian

$$H=-2J\sum_{(i,j)}p_ip_j\mathbf{S}_i\cdot\mathbf{S}_j\ , \tag{2.1}$$

where $J>0$ and (i,j) denote the nearest-neighbor pairs defined on a magnetic site-dilute cubic lattice. The p_i's are random site variables taking the values 1 and 0 with probability p and $1-p$, respectively. The ground state of Eq. (2.1) is the ferromagnetic $|0\rangle$ state and we can write the Schrödinger equation for a state $|\Psi\rangle$ corresponding to a single spin deviation so that the total z component of the crystal spin is one unit less. The wave function $|\Psi\rangle$ is expanded in the Hilbert space basis set which consists of one-particle spin deviations defined on every lattice site n, that is

$$|\Psi\rangle=\sum_n\Psi_n|n\rangle\ , \tag{2.2}$$

where $|n\rangle=(2S)^{-1/2}S_n^-|0\rangle$. If we set $2JS=1$ the equation studied can be derived from an equivalent general tight-binding Hamiltonian

$$H=\sum_n\varepsilon_n|n\rangle\langle n|+\sum_{(n,m)}|n\rangle\langle m|\ . \tag{2.3}$$

In this case n covers all the existing magnetic lattice sites on a three-dimensional lattice and (n,m) denotes all present nearest-neighbor pairs of connected sites. The site-energy ε_n is equal to the number of nearest neighbors of n present which ranges from 0 to 6 for a simple cubic lattice. The model has a special form of correlated disorder between the diagonal and off-diagonal matrix elements. The energies are measured from the ground state and the gapless spectrum consists of strictly positive energies confined within the energy interval $0\le E\le 12$. The $E=0$ mode is extended, even in the presence of site randomness, due to the continuous degeneracy of the ground state.

At the critical percolation concentration p_c ($p_c\approx 0.31$ for a *sc* lattice in $d=3$) the excitations are known as fractons,[2] due to the underlying fractal nature of the cluster. The fracton states are expected to persist at any concentration for small enough length scales restricted by the percolation correlation length. The density of states for the fracton spectrum at p_c shows a divergence for long wavelengths following the universal Alexander-Orbach law:[2]

$$\rho(E)\propto E^{d_f/d_w-1},\quad E\to 0\ . \tag{2.4}$$

The exponent d_f is the fractal dimension which takes the value $d_f\approx 2.51$ (Ref. 1) for the three-dimensional percolating cluster and d_w is the dynamical exponent following from the obeyed anomalous dispersion $E\propto k^{d_w}$ for $k\ll 1$. If we cast Eq. (2.4) into the usual form of the magnon density of states then

$$\rho(E)\propto E^{(d_s-2)/2},\quad E\to 0\ , \tag{2.5}$$

and the relevant exponent which plays the role of the space dimension is now $d_s=2d_f/d_w$, better known as the fracton or spectral dimension. It has been conjectured that d_s takes approximately its mean-field value ($d_s\approx\frac{4}{3}$) in any Euclidean dimension $d\ge 2$.[2] For concentrations above p_c the magnon density of states is observed in the long-wavelength (small-E) regime while a crossover to the fracton regime occurs at shorter wavelengths (larger-E). The magnon-fracton crossover is expected at a characteristic energy which is inversely proportional to the percolation correlation length. The Alexander-Orbach conjecture as suggested by Eq. (2.4) has been numerically verified in two dimensions[8–10] where the magnon-fracton crossover was found to be smooth.[10] The absence of such studies in three dimensions was the main motivation for the present work.

III. CALCULATIONS

A. The moments

Firstly, we focused on the density of states problem for the site-dilute ferromagnet in a cubic lattice as a function of the concentration p by evaluating exactly its first ten frequency moments. We have used the already known moments for the k-dependent spectral functions of Ref. 11 calculated by a variant of a finite-cluster method.[12] In order to obtain the moments of the density of states we must integrate the k-dependent expressions of Ref. 11 over all k vectors in the first Brillouin zone. In fact, we evaluated integrals for the different powers of functions containing the following lattice expressions:[11]

$$\begin{aligned}\varepsilon_1&=6-2[\cos(\pi k_x)+\cos(\pi k_y)+\cos(\pi k_z)]\ ,\\ \varepsilon_2&=12-4[\cos(\pi k_x)\cos(\pi k_y)+\cos(\pi k_y)\cos(\pi k_z)\\ &\quad+\cos(\pi k_z)\cos(\pi k_x)]\ ,\\ \varepsilon_3&=8-8[\cos(\pi k_x)\cos(\pi k_y)\cos(\pi k_z)]\ ,\end{aligned} \tag{3.1}$$

which enter in the k-dependent moments. We have done this efficiently by expanding the corresponding powers and a list of the obtained first ten moments as a function of the percolation concentration p is analytically given in Table I. For the pure lattice limit the moments we obtain

TABLE I. The first ten moments of the one-magnon density of states for the site dilute lattice in $d=3$ as a function of the concentration p.

Order	Moment
0	1
1	$6p$
2	$12p+30p^2$
3	$24p+180p^2+120p^3$
4	$48p+750p^2+1524p^3+360p^4$
5	$96p+2700p^2+11\,040p^3+8880p^4+720p^5$
6	$192p+9030p^2+62\,556p^3+102\,690p^4+38\,424p^5+864p^6$
7	$384p+28\,980p^2+310\,464p^3+850\,332p^4+683\,952p^5+140\,856p^6+3264p^7$
8	$768p+90\,750p^2+1\,423\,548p^3+5\,853\,432p^4+7\,902\,360p^5+3\,703\,872p^6+587\,712p^7+39\,792p^8$
9	$1536p+279\,900p^2+6\,207\,888p^3+35\,964\,000p^4+72\,073\,536p^5+57\,150\,264p^6+19\,461\,960p^7$ $+3\,410\,688p^8+337\,200p^9$
10	$3072p+855\,030p^2+26\,193\,900p^3+205\,138\,440p^4+567\,549\,156p^5+663\,580\,182p^6+372\,219\,936p^7$ $+113\,727\,048p^8+24\,234\,792p^9+2\,112\,096p^{10}$

are given in Table II. If these results are transformed for the corresponding tight-binding electron problem in a dilute lattice, better known as the quantum percolation model, they agree for $p=1.0$ with the results of Ref. 13.

B. The moments maximum-entropy method

The integrable and non-negative $\rho(E)$ is the required quantity which is defined for E on the interval [0,12]. Our purpose is to achieve the evaluation of the density of states when a small number of its moments is known. Suppose that the following N moments

$$\mu_m=\int \rho(E)E^m dE, \quad m=0,1,\ldots,N \ , \tag{3.2}$$

are known. The maximum-entropy solution is a density $\rho(E)$ which maximizes the entropy functional $-\int \rho(E)\ln[\rho(E)]dE$, under the constraints of Eq. (3.2). According to Ref. 5 a unique maximum-entropy solution exists of the form

$$\rho(E)=\exp\left[\sum_{m=0}^{N}\lambda_m E^m\right] . \tag{3.3}$$

The values of the parameters λ_m are chosen so that they satisfy the constraints of Eq. (3.2) by calculating and subsequently minimizing the function

TABLE II. Moments of the one-magnon density of states for the ordered lattice ($p=1.0$) in $d=3$.

Ord	er	Moment
	0	1
	1	6
	2	42
	3	324
	4	2682
	5	23 436
	6	213 756
	7	2 018 232
	8	19 602 234
	9	194 886 972
	10	1 975 613 652

$$\int \exp\left[\sum_{m=0}^{N}\lambda_m E^m\right]dE-\sum_{m=0}^{N}\mu_m\lambda_m \ .$$

A numerical procedure of how to do this efficiently, at least for not too many moments, is given in Ref. 5. The λ_m's are numerically obtained by inverting a Hessian matrix and $\rho(E)$ is recovered from Eq. (3.3). In our application we have used as input the moments given in Table I. The results are displayed in Figs. 1–3.

C. The exact diagonalization approach

In order to complement and back up our calculations we have also used a more accurate but cumbersome approach. We generate numerically a statistical ensemble of randomly dilute finite cubic lattices using periodic boundary conditions in every direction. The corresponding one-magnon Hamiltonian matrices were set up and diagonalized numerically as it was done before for $d=2$.[8–10] To calculate $\rho(E)$ for a particular value of p all the eigenvalues were computed. Their distribution density is shown in histogram form for various concentrations p in Figs. 1 and 2 compared with the moments maximum-entropy results. The lattice size for most calculations is $14\times14\times14$. In this type of calculation there exist two sources of error. Firstly, a statistical error arises due to the finite number of samples considered in taking the average. We estimated the relative statistical fluctuations for the number of states in every bin and was found to be no more than about 6%. Finite-size effects are also unavoidable and become noticeable in the figures particularly for low disorder, since every bin contains a rather small number of states. In order to estimate the errors from this source we tried varying the lattice size. In Figs. 1(a) and 1(b) we present averages in a histogram form for two different lattice sizes which give an estimate of the total error.

IV. RESULTS

The results of our calculations by both the methods described above are demonstrated in Figs. 1–4. The nor-

malized $\rho(E)$, as p approaches p_c, is seen to display the well-known δ function singularity peaks containing highly degenerate eigenstates. The most prominent peak occurs at $E=0$ but peaks at $E=1,2,3,(3+\sqrt{5})/2,\ldots$, can be also seen causing a rapid increase in the number of states in the corresponding energy bins. A sufficient explanation on the origin of these special states is given in Ref. 14 for the related quantum percolation model. They are due to states localized both on small isolated clusters as well as special parts of the infinite percolating cluster. Their degeneracy ratio can be evaluated by cluster-counting procedures and for $p=p_c$ we numerically find that the $E=0$ states consist of $\approx 17\%$ of the total number of states. At the percolation threshold (Fig. 1) we obtain a divergence at long wavelengths as expected from Eqs. (2.4) and (2.5). It can be seen that the results obtained by the maximum-entropy method compare reasonably well with the detailed numerical data (see Fig. 2). Difficulties arise when one tries to improve the comparison mostly due to the presence of δ-function singularities which are not maximum-entropy but instead minimum-entropy solutions. For higher p values the significance of the δ functions diminishes and the maximum-entropy method becomes very good. Even for the regular-cubic-lattice limit, which is highly unsuitable for this kind of approach, the maximum entropy using ten moments is reasonable. In Fig. 3 the regular lattice density of states is recovered,[4] with the square-root behavior for low E, although finite-moment effects result in positive $\rho(E)$ values at the band edges. The agreement is improved when more moments are considered.

In order to discuss the fracton excitations due to the percolating cluster at p_c we consider the numerically computed integrated density of states $N(E)$. In Fig. 4 we plot $N(E)$ against E in a double logarithmic plot. In the energy range considered there is no significant number of degenerate eigenstates. We expect from Eq. (2.5) that in the fracton regime the data should lie on a straight line of slope $d_s/2$. In the magnon regime the square-root law for $\rho(E)(\propto E^{1/2})$ suffices and results in $N(E)\propto E^{3/2}$, which means that d_s takes the value of the space dimen-

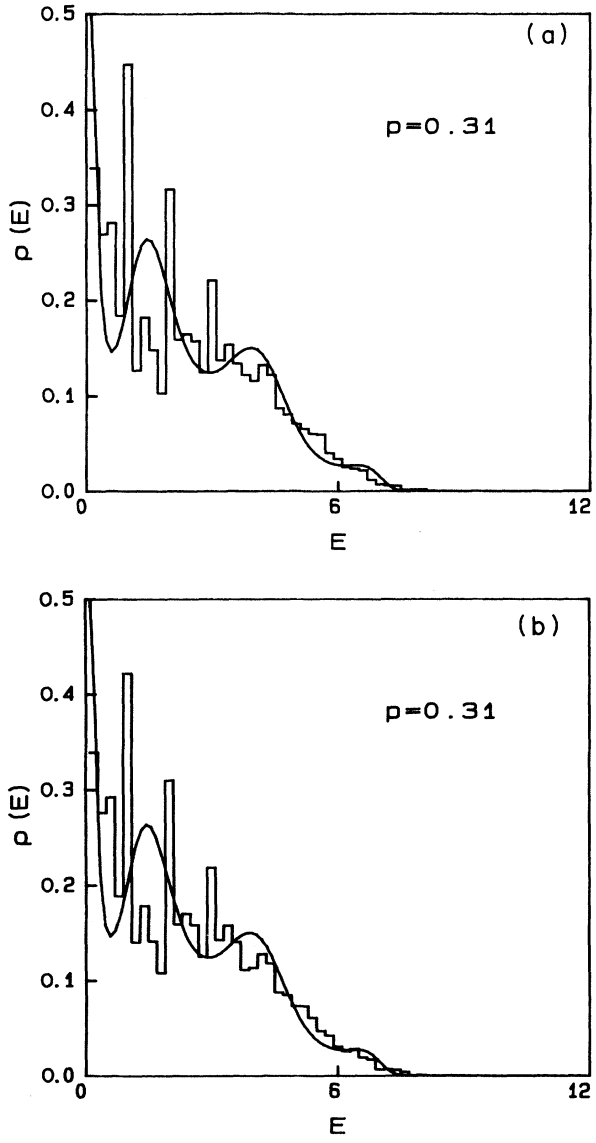

FIG. 1. (a) The averaged normalized one-magnon density of states is displayed at the critical percolation concentration $p_c=0.31$. The continuous line is the result by the maximum-entropy method using the first eight moments via Table I. The histogram is obtained from a direct finite lattice ($14\times14\times14$) exact numerical diagonalization. The average is taken over 20 random configurations. The large peaks correspond to δ-function singularities (see text) which occur at special energies. The peak containing states in the range $0\le E<0.1$ is not shown. (b) The same as in (a) but the histogram is now obtained by diagonalizing a smaller lattice ($12\times12\times12$) and the average is taken over 50 random samples.

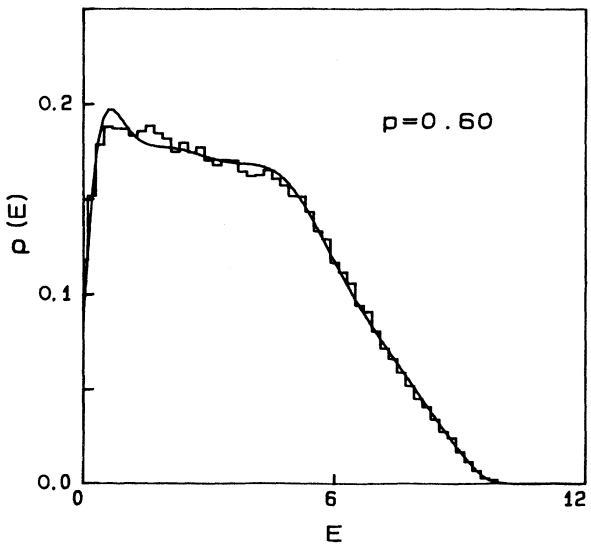

FIG. 2. The histogram is of the density of states for $p=0.6$ [as in Fig. 1(b)]. The continuous line gives the corresponding result of the moments maximum-entropy method using the ten moments of Table I.

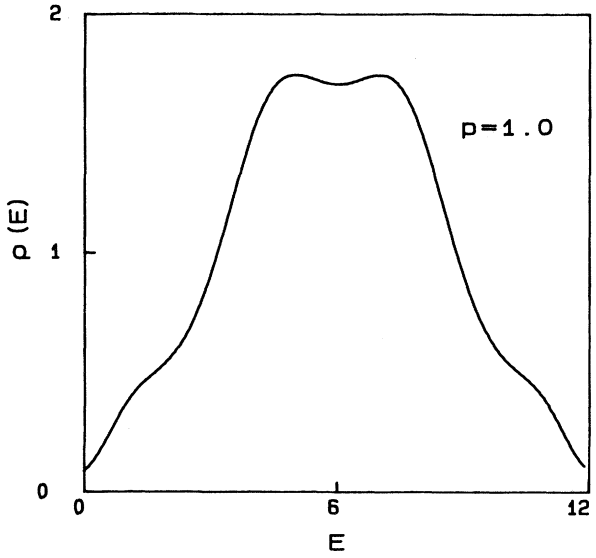

FIG. 3. Plot of the moments maximum-entropy method result for the density of states of the ordered cubic lattice using the ten moments ($p=1.0$) of Table II.

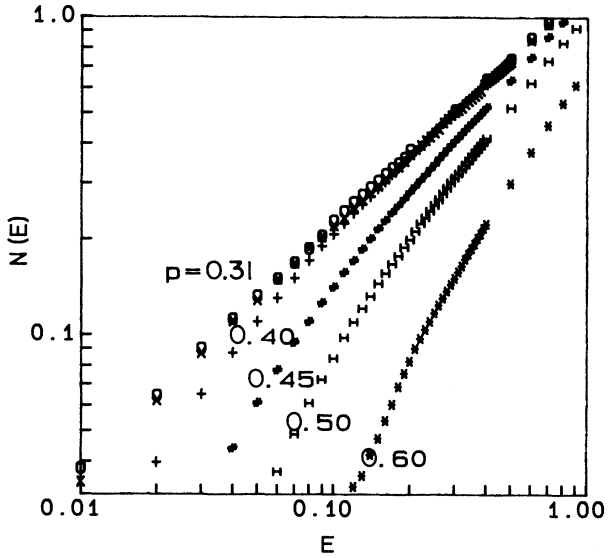

FIG. 4. log-log plot of the averaged normalized integrated density of states $N(E)$ vs energy E. From Eq. (2.5) $N(E) \propto E^{d_s/2}$ and the crossover from the magnon ($d_s=d=3$) to fracton ($d_s \approx 4/3$) (Ref. 2) excitations can be seen for $p > p_c$. The obtained value for the exponent d_s is $d_s = 1.52 \pm 0.05$ at all low enough energies for $p = p_c$ and only at the higher energy part of the spectrum for $p_c < p < 1$ (fracton regime). From the present data it can be concluded that $\rho(E)$ varies smoothly at the crossover.

sion $d=3$. For $p=p_c$ despite the various sources of error the data lie approximately on a straight line and a least-squares fit gave a gradient leading to a value of $d_s = 1.52 \pm 0.05$. The error bound is estimated from performing various runs and contains both the statistical and finite-size components. Our results for d_s are small overestimates in respect to the nearly universal value of $\frac{4}{3}$. For values of p above p_c the two excitation regimes are seen to be roughly characterized by the corresponding exponents d_s and d, respectively. Our results show no indication of a well-defined fracton peak, although a smooth curvature of the data is seen at the crossover. By the maximum-entropy method we fail to obtain a very accurate value for the exponent d_s. This is due to the fact that in the method we cannot eliminate the degenerate δ functions already present in the input moments. However, the divergence of $\rho(E)$ at low E is seen and a d_s close to the previous value can be extracted. For wavelengths longer than the scale of dilution the pure density law $\rho(E) \propto E^{(d-2)/2}$ is obtained by this technique. In Fig. 2 for $p=0.6$ the difference from p_c is high enough but a small peak in the density of states at small E is seen even in the gross scale of the figure which may be due to the magnon-fracton crossover in $d=3$.[15] We can conclude that for most disordered systems the maximum-entropy technique becomes very powerful, even when a few moments are used.

The fracton states are expected to have interesting localization properties[16,17] such as the occurrence of superlocalization.[18] From our preliminary numerical data the scaling of the moments for the wave-function amplitude distributions implies superlocalization of the fracton states as in $d=2$.[19] We hope to consider this question in a future publication.

V. DISCUSSION

The results of this paper should also apply to the problem of vibrational density of states if E is replaced by the squared phonon frequency ω^2. The steep change in the density of states (see Fig. 2) is also found in the original effective medium treatments.[15] The present results become relevant for the specific-heat density of states in glasses[20] and neutron-irradiated quartz. Equilibrium properties of adsorbed films also should depend on the spectral dimension of the substrate following recent discussions of Bose-Einstein condensation in porous systems.[21]

In conclusion, a moments maximum-entropy method is presented here as an alternative powerful tool for calculating densities of states in disordered systems together with the more cumbersome direct finite-size lattice numerical method. We are able to recover the basic theoretical results concerning the spectra of magnon excitations on random fractal networks in $d=3$, limited so far only to effective medium treatments. Our results are in favor of the fracton interpretation in amorphous systems. Clearly more work is needed on two fronts: firstly, on the improvement of the method for more accurate studies, also by including a larger number of moments and extending the range of applications to other complicated spectral problems in disordered systems.

ACKNOWLEDGMENTS

Thanks are due to Professor N. Papanicolaou of the Research Center of Crete (see also Ref. 5 and please note that one of us has the same name) for helpful discussions and for allowing us to use his numerical program for the evaluation of the spectral density and Dr. R. Djordjevic who initially helped us with the calculation of the first few moments. The work was also supported in part by a II.EN.E. Δ. Grant from the Greek Secretariat of Science and Technology.

---

[1]D. Stauffer, *Introduction to Percolation Theory* (Taylor and Frances, London, 1985).
[2]S. Alexander and R. Orbach, J. Phys. (Paris) Lett. **43**, L625 (1982).
[3]A. B. Harris, P. L. Leath, B. G. Nickel, and R. J. Elliot, J. Phys. C **7**, 1693 (1974).
[4]E. N. Economou, *Green's Functions in Quantum Physics,* Springer Verlag Series in Solid State Physics, Vol. 7 (Springer, New York, 1983).
[5]L. R. Mead and N. Papanicolaou, J. Math. Phys. **25(8)**, 2404 (1984).
[6]E. T. Jaynes, Phys. Rev. **106**, 620 (1957); **108**, 171 (1957).
[7]P. A. Fedders and A. E. Carlsson, Phys. Rev. B **32**, 229 (1985).
[8]S. J. Lewis and M. C. O'Brien, J. Phys. C **18**, 4487 (1985).
[9]S. J. Lewis and R. B. Stinchcombe, Phys. Rev. Lett. **52**, 1021 (1984).
[10]S. N. Evangelou, Phys. Rev. B **33**, 3602 (1986).
[11]B. Nickel, J. Phys. C **7**, 1719 (1974).
[12]C. Domb, Adv. Phys. **9**, 149 (1960).
[13]M. E. Fisher and W. J. Camp, Phys. Rev. B **5**, 3730 (1972).
[14]S. Kirpatrick and T. P. Eggarter, Phys. Rev. B **6**, 3598 (1972).
[15]B. Derrida, R. Orbach, and Kin-Wah Yu, Phys. Rev. B **29**, 6645 (1984).
[16]R. Rammal and G. Toulouse, J. Phys. (Paris) Lett. **44**, 13 (1983).
[17]I. Webman and G. S. Grest, J. Phys. (Paris) Lett. **44**, L1155 (1984).
[18]Y. E. Levy and B. Souillard, Europhys. Lett. **4**, 1233 (1987).
[19]T. Nakayama, K. Yakubo, and R. Orbach J. Phys. Soc. Jpn. **58**, 1891 (1989).
[20]S. Alexander, C. Laermans, R. Orbach, and H. M. Rosenberg, Phys. Rev. B **28**, 4615 (1983).
[21]P. Pfeifer and M. Order, in *The Fractal Approach to Heterogeneous Chemistry,* edited by D. Avnir (Wiley, Chichester, England, 1989), pp. 11–43.