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Dispersionless states in random Cayley trees with multiple connectivity

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Exponentially localized states appear at the center of the energy spectrum of Cayley trees characterized by two different connectivities randomly distributed within the tree. These states share with "ultralocalized" states (states located on a few sites of the lattice) found in dilute lattices and, more recently, in Penrose lattices the surprising feature of showing no dispersion. This random system illustrates the fact that disorder not always tends to round off the density-of-states curves or to broaden δ-function peaks.

Solid-state physics presents many examples of band-center singularities when simple tight-binding Hamiltonians are employed to model physical systems. Paradigms are the logarithmic Van Hove singularity appearing in the density of states of a two-dimensional square lattice[1] and the δ-function peak appearing in the gap of the density of states of a dilute cubic lattice.[2] The origin of the singular behavior is quite different in both cases. While the Van Hove singularity describes extended states in an infinite periodic lattice, the Kirkpatrick-Eggarter singularity comes from "ultralocalized" states in a disordered system. A noncomprehensive list of some further examples is given in Ref. 3. Very recently, Penrose lattices (two-dimensional quasicrystals) have added a new example to this kind of singular behavior, and, as a consequence, new contributions to the subject have appeared.[4-6] It seems clear[7] now that a great variety of systems formed by two atomic species with different coordinations show "ultralocalized" states. We report in this paper the results of a study of this phenomenon in Cayley trees characterized by two different connectivities randomly distributed within the tree. Our analysis extends the knowledge of band-center singularities to random systems that can be studied very precisely both numerically and analytically due to their inherent simplicity.[8] As a by-product of our work, we test further an analytical approximation that reproduces very accurately the density of states of complex random Cayley trees obtained by computer simulation. These complex Cayley trees have been used to study the electronic structure of amorphous semiconductor alloys.[9]

We study a stoichiometric binary alloy $A_{x_A}B_{x_B}$ formed by A atoms (atoms linked to k_A+1 first neighbors) and B atoms (atoms linked to k_B+1 first neighbors). A forms A—A and A—B bonds with probabilities 1-p and p, respectively, whereas B forms B—A and B—B bonds with probabilities q and 1-q, respectively. Equalizing the number of crossed bonds obtained starting from A or B atoms, we have

$$x_A(k_A+1)p=x_B(k_B+1)q \ , \tag{1}$$

which together with the stoichiometric requirement

$$x_A(k_A+1)=x_B(k_B+1) \tag{2}$$

implies the equality of crossed probabilities:

$$p=q \ . \tag{3}$$

The probability p is related to the atomic correlation that takes place in the binary alloy. It varies from $p=0$ (there are no crossed bonds; A and B form separate phases) to $p=1$ (all tree branches show perfect atomic alternation $\ldots ABABAB\ldots$). One s orbital per site is considered. Atomic energies are equal to zero for both A and B atoms and all first-neighbor interactions are equal to V. Local properties of random Cayley trees are determined completely by two sets of complex energy-dependent self-energies $\{\Sigma_A(E)\}$ and $\{\Sigma_B(E)\}$ acting on sites A and B, respectively. The probability distributions of self-energies are governed by the following probabilistic equations:

$$\Sigma_A(E)=V^2\bigg/\left[E-E_t-\sum_{i=1}^{k_t}\Sigma_t(E)\right] , \tag{4a}$$

$$\Sigma_B(E)=V^2\bigg/\left[E-E_t-\sum_{i=1}^{k_t}\Sigma_t(E)\right] , \tag{4b}$$

where t is a random subindex that takes values A and B with probabilities 1-p and p, respectively, in Eq. (4a) and that takes values A and B with probabilities p and 1-p, respectively, in Eq. (4b). Also $\Sigma_A(E)$ and $\Sigma_B(E)$ are random variables that take values according to their distributions $\{\Sigma_A(E)\}$ and $\{\Sigma_B(E)\}$. Equations (4a) and (4b) show that the difference between $\{\Sigma_A(E)\}$ and $\{\Sigma_B(E)\}$ stems from the difference in the distribution of atomic configurations about A and B atoms, or in other words, only the difference in the subindex distribution makes a difference between both equations. Finite distributions of self-energy values are obtained numerically through iteration of Eqs. (4a) and (4b). We have checked that final self-energy distributions are independent from initial self-energy values whenever the number of iterations is large enough. Typical values of the computational parameters are 1000 self-energy values in each set, 75 iteration loops and $\mathrm{Im}E=0.01\,|\,V\,|$. Some tests with different values of the parameters have been run to obtain an estimate of the achieved numerical precision.

Once the self-energy distributions $\{\Sigma_A(E)\}$ and

$\{\Sigma_B(E)\}$ are known, local densities of states are given by:

$$N_A(E)=-(1/\pi)\mathrm{Im}\left\{E-\sum_{i=1}^{k_A+1}\Sigma_A(E)\right\}^{-1}, \tag{5a}$$

$$N_B(E)=-(1/\pi)\mathrm{Im}\left\{E-\sum_{i=1}^{k_B+1}\Sigma_B(E)\right\}^{-1}. \tag{5b}$$

Finally, an average over atomic configurations, i.e., over $\{\Sigma_A(E)\}$ and $\{\Sigma_B(E)\}$, allows the obtention of the averaged local densities of states on atoms A and B, respectively.

Following previous work,[8,9] analytical approximations for the averaged local densities of states are obtained by means of a self-consistent definition of two effective mediums $\Sigma_A(E)$ and $\Sigma_B(E)$. (Note that we are using the same notation for the self-energies in spite of the change of character of the variables.) The first (one-step) approximation to the effective mediums is determined by the following equations:

$$\{E-(k_A+1)\Sigma_A(E)\}^{-1}=(1-p)\{E-k_A\Sigma_A(E)-V^2/(E-k_A\Sigma_A(E))\}^{-1}+p\{E-k_A\Sigma_A(E)-V^2/(E-k_B\Sigma_B(E))\}^{-1}, \tag{6a}$$

$$\{E-(k_B+1)\Sigma_B(E)\}^{-1}=(1-p)\{E-k_B\Sigma_B(E)-V^2/(E-k_B\Sigma_B(E))\}^{-1}+p\{E-k_B\Sigma_B(E)-V^2/(E-k_A\Sigma_A(E))\}^{-1}. \tag{6b}$$

Equations (6a) and (6b) are usually inverted to obtain $\Sigma_A(E)$ and $\Sigma_B(E)$ as a function of $\Sigma_A(E)$ and $\Sigma_B(E)$, and then, they can be solved iteratively. We have taken the imaginary part of E equal to zero in the last part of the iteration procedure. In this way, the appearance of gaps is unambiguously shown by the calculated density of states.

Further approximations to the effective media $\Sigma_A(E)$ and $\Sigma_B(E)$ are obtained through averages over larger atomic configurations that are generated by two or more steps along branches of the Cayley tree. (See Ref. 8 for a systematic comparison of analytical approximations done to study diluted Cayley trees.) We have verified that the two-step approximation is good enough for the system under study. Furthermore, the one-step approximation is as good as this except for energies around $E=0$. The self-consistent equations for the two-step approximation are not given here because their form depends explicitly on the connectivities. (Note that both the two-step configurations used to define the effective medium and their probabilities do depend on the Cayley-tree connectivities.) Nevertheless, they can be very easily derived by the interested reader.

At the end of this paper we will compare our analytical approximations with the Kittler-Falicov analytical method.[10] For the sake of completeness, we write the equations that give the effective medium in this scheme:

$$\Sigma_A(E)=(1-p)V^2/(E-k_A\Sigma_A(E))+pV^2/(E-k_B\Sigma_B(E)), \tag{7a}$$

$$\Sigma_B(E)=pV^2/(E-k_A\Sigma_A(E))+(1-p)V^2/(E-k_B\Sigma_B(E)). \tag{7b}$$

Through these equations, a direct average over the self-energies corresponding to one-step atomic configurations is done. Their relationship with the exact probabilistic Eqs. (4a) and (4b) is evident. This averaging procedure can be contrasted with the one done using the diagonal elements of the Green function [Eqs. (6a) and (6b)].

Once the effective media have been obtained, averaged local densities of states are given by

$$N_A(E)=-(1/\pi)\mathrm{Im}[E-(k_A+1)\Sigma_A(E)]^{-1}, \tag{8a}$$

$$N_B(E)=-(1/\pi)\mathrm{Im}[E-(k_B+1)\Sigma_B(E)]^{-1}. \tag{8b}$$

In addition, more complex atomic configurations can be studied by saturating the configuration by the corresponding effective media (cluster-Bethe-lattice calculations in a widely used nomenclature).

We have applied the preceding methods to the study of Cayley trees with two different kinds of branching defined by connectivities $k_A=1$ and $k_B=4$. Our results for the averaged local density of states as a function of p are compiled in Figs. 1 and 2. In these figures both "exact" numerical results and approximate analytical results are shown. We start the discussion by analyzing the two extreme values $p=0$ and $p=1$. The case $p=0$ is trivial: two separate Cayley trees of connectivities 1 and 4 give rise to well-known densities of states with band limits $\pm 2V$ and $\pm 4V$, respectively. The value $p=1$ originates a regular Cayley tree with alternating branching. This tree is exactly solvable. The continuous part of the local density of states on an atom of connectivity k is given by

$$N_k(E)=(1/\pi)k(k+1)[-E^4+2(k+k')V^2E^2-(k-k')^2V^4]^{1/2}/\{(k+1)^2[(k^2-1)(k'-k)+k+k']V^2-2kE^2\}\,|E|\,, \tag{9}$$

where k' is the second connectivity of the ordered Cayley tree ($k'=k_B$ for $k=k_A$ and $k'=k_A$ for $k=k_B$). The spectrum is formed by four bands with limits which are $\pm(\sqrt{k_B}\pm\sqrt{k_A})V$. In addition to the continuous part of the spectrum there is a δ function at the gap center ($E=0$) on the sites of smaller connectivity (A sites). Its weight is $(k_B-k_A)/(k_B+1)$. (In Figs. 1 and 2 the spectrum for $k_A=1$ and $k_B=4$ is shown. The energies of the

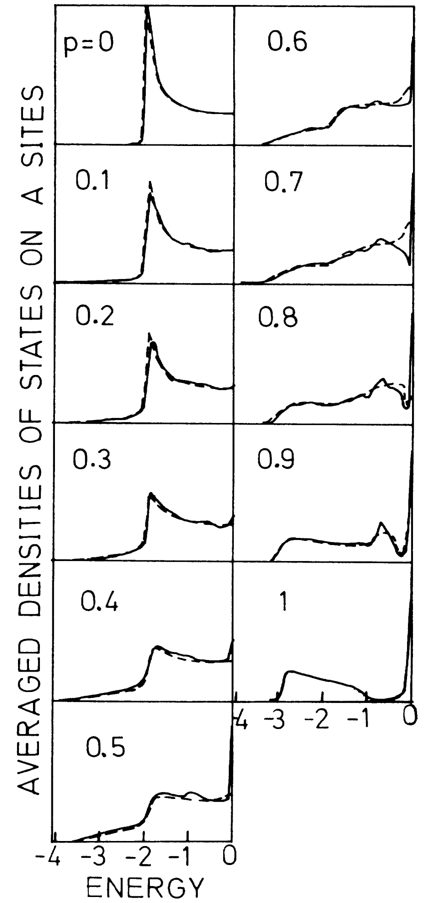

FIG. 1. Averaged densities of states on A sites ($k_A=1$) as a function of p [the probability that an A (B) site is connected to a B (A) site] in a random Cayley tree with two different connectivities $k_A=1$ and $k_B=4$. Numerical results obtained by simulation, solid line, are compared with an analytical approximation, dashed line. With the spectra symmetric about $E=0$, only the right parts of them are shown. The energy scale ranges from $-4.1|V|$ to 0 and the density-of-states scale ranges from 0 to $0.7|V|^{-1}$.

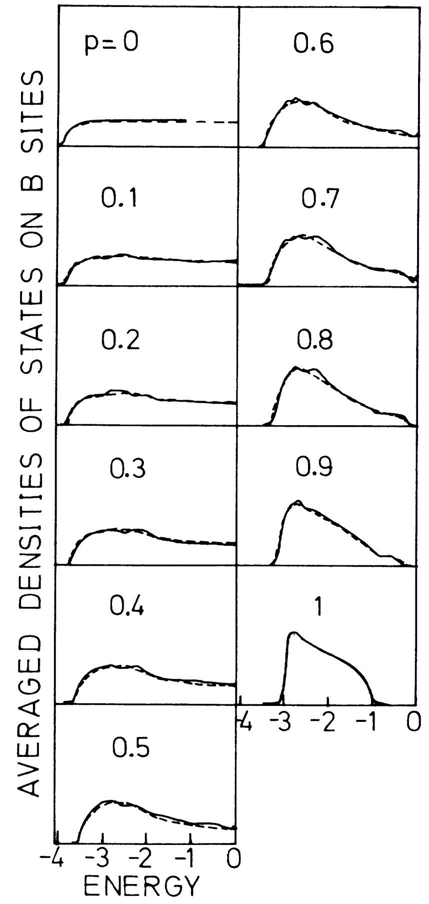

FIG. 2. Averaged densities of states on B sites ($k_B=4$) as a function of p [the probability that an A (B) site is connected to a B (A) site] in a random Cayley tree with two different connectivities $k_A=1$ and $k_B=4$. See also the caption of Fig. 1.

band edges are at $\pm 3V$ and $\pm V$ for these connectivities.)

It is interesting to obtain the wave function of the localized state. To this end, linear combinations of orbitals with spherical symmetry around the central A atom are considered. Let $c_0, c_1, c_2, \ldots$ be the coefficients of the wave function in terms of the symmetrized linear combinations of orbitals located on shells $0,1,2,\ldots$. Application of Schrödinger equation gives the following set of equations:

$$\begin{aligned} Ec_0 &= \sqrt{k_A+1}\,c_1 ,\\ Ec_1 &= \sqrt{k_A+1}\,c_0 + \sqrt{k_B}\,c_2 ,\\ Ec_2 &= \sqrt{k_B}\,c_1 + \sqrt{k_A}\,c_3 ,\\ Ec_3 &= \sqrt{k_A}\,c_2 + \sqrt{k_B}\,c_4 ,\\ Ec_4 &= \sqrt{k_B}\,c_3 + \sqrt{k_A}\,c_5 ,\\ Ec_5 &= \sqrt{k_A}\,c_4 + \sqrt{k_B}\,c_6 . \end{aligned} \tag{10}$$

The wave function corresponding to $E=0$ is easily obtained from Eqs. (10):

$$\begin{aligned} c_1 &= c_3 = c_5 = \cdots = 0 ,\\ c_2 &= -\sqrt{(k_A+1)/k_B}\,c_0 ,\\ c_4 &= \sqrt{k_A/k_B}\sqrt{(k_A+1)/k_B}\,c_0 ,\\ c_6 &= -(k_A/k_B)\sqrt{(k_A+1)/k_B}\,c_0 . \end{aligned} \tag{11}$$

Finally, normalization of the wave function requires that $c_0=[(k_B-k_A)/(k_B+1)]^{1/2}$ and the wave function coefficients become specified. Thus, there is an exponentially localized state of localization length λ given by

$$\lambda = 2/\ln(k_B/k_A) \tag{12}$$

in terms of steps along branches of the Cayley tree. Further localized states with similar properties are obtained for different symmetries. Nevertheless, these states do not contribute to the density of states on the central atom. (Only states with spherical symmetry contribute to the density of states on the central atom of a Cayley tree when one s orbital per site is considered in the Hamiltonian.) In conclusion, the δ-function peak at the band center comes from a "nondispersive band" of exponentially localized states. Neither extended states as it happens for Van Hove singularities,[1] nor "ultralocalized" states as they appear in dilute lattices[2] are responsible for the band-center singularity. In some sense, the system under study constitutes an intermediate example between well-known extremes.

The Cayley tree of alternating branching falls into the category of systems for which Sutherland's theorem[7] is applicable. The following properties are correctly predicted by the theorem. The spectrum is symmetric about $E=0$ and it has a δ-function peak of finite weight at the spectrum center [$|k_A-k_B|/(k_A+k_B+2)$ is the average weight for the regular Cayley tree]. Localized states are confined to one of the sublattices, to the sites of smaller coordination in this case.

Following now our numerical results (Figs. 1 and 2) from $p=1$ to $p=0$, we note that the bands broaden and the gap disappears around $p=0.7$. These features are easily understandable in terms of the $p=0$ case. Nevertheless, the most interesting facts occur in the neighborhood of $p=1$ before the gap around $E=0$ closes. Figures 1 and 2 show that for $p<1$ new bands around $E=\pm 0.7V$ appear *but the central peak does not broaden.* This is our main numerical result. We have checked this assertion by a study of the dependence of the peak height on the imaginary part of the energy. The study reveals a δ-function peak behavior.

We have studied the $p \rightarrow 1$ limit in order to understand the effect of disorder for $p<1$. In this limit the principal defects occurring in the Cayley tree are local failures of alternation, i.e., the appearance of . . . *ABABAABAB*. . . and . . . *ABABBABAB*. . . paths along the branches of the Cayley tree. For $p \rightarrow 1$, it suffices to study one isolated defect of each of these two types. We have found that the first type of defects explains our numerical results. A . . . *ABABAABAB*. . . defect removes two states from the peak at $E=0$ and produces two new localized states at $E=\pm 0.7V$. Furthermore, it can be checked directly that the rest of the states belonging to the central peak do change their wave function without changing their energy. Figure 3 shows one of the new states at $E=0$ in order to illustrate the phenomenon. Isolated defects do not produce states of energy very close to 0 and, therefore, the central peak does not broaden for $p \rightarrow 1$.

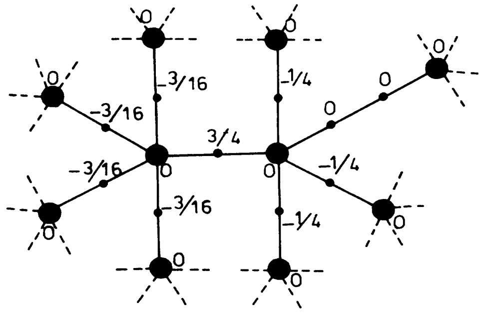

FIG. 3. Example of a wave function of zero energy in a perfectly alternating Cayley tree with a defect of the . . . *ABABAABAB*. . . type.

Finally, we will briefly comment on the analytical approximations to the spectra of random Cayley trees. As the comparison done in Figs. 1 and 2 proves, the analytical approximation reproduces very well the numerical results except in the neighborhood of $E=0$. While numerical results show the permanence of the δ-function peak until $p \approx 0.5$, the central peak disappears from the analytical approximation for $p<0.8$, just when the gap closes. A deeper analysis shows that the central peak is given by our approximation as an extremely narrow band instead of as a δ function. Figure 4 shows that this failure is largely magnified by the standard Kittler-Falicov approximation.[10]

As a summary of our work, the following results can be remarked.

(i) Regular Cayley trees with alternating connectivities show exponentially localized states at the spectrum center within the gap opened by the alternating connectivity.

(ii) The peak in the density of states that describes these localized states does not broaden when perfect alternation disappears.

(iii) This behavior can be easily understood in the quasi-perfect limit. Wave functions are able to adapt themselves to the defects without changing their energy.

(iv) An analytical approximation to the density of states reproduces the numerical results quite satisfactorily.

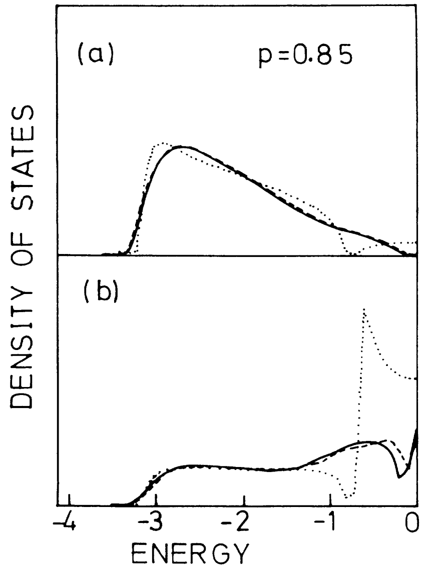

FIG. 4. Comparison of three analytical approximations for the case $p=0.85$. (i) Two-step analytical approximation shown in Figs. 1 and 2 together with the numerical results, solid line; (ii) one-step analytical approximation defined by Eqs. (6a) and (6b), dashed line; and, (iii) Kittler-Falicov analytical approximation defined by Eqs. (7a) and (7b), dotted line. (a) shows the averaged density of states on B sites, whereas (b) shows the averaged density of states on A sites. Scales as in Figs. 1 and 2.

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