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RENORMALIZATION GROUP DECIMATION TECHNIQUE FOR DISORDERED BINARY HARMONIC CHAINS *

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ABSTRACT

The density of states of disordered binary harmonic chains is calculated using the Renormalization Group Decimation technique on the displacements of the masses from their equilibrium positions. The results are compared with numerical simulation data and with those obtained with the current method of Goncalves da Silva and Koiller. The advantage of our procedure over other methods is discussed.

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In a recent paper [1] a systematic procedure for the calculation of spectra of elementary excitations, wave functions and density of states with the Renormalization-Group (RG) decimation technique was proposed. The method is exact for 1-d problems with nearest neighbours interaction which have or have not the translational invariance. In these models the philosophy of the RG, which is to change a problem with many degrees of freedom into another one with less degrees of freedom without losing any physical feature, can be fulfilled without any approximation. Several physical systems of recent interest can be described by those models: crystals containing a modulating periodic potential of a period different from that of the underlying lattice, either conmensurate or inconmensurate with it [2], electrons in 2-d square lattice in a perpendicular magnetic field [3], the Schrödinger equation with an arbitrary potential of atomic type (through the construction of the Poincaré map of the problem [4]), superconductive networks (through the De Gennes-Alexander theory [5]) etc.

The method starts with the equation of motion for the wave function, order parameter, etc., depending on the problem. Next, the intermediate degrees of freedom are eliminated obtaining the equation of motion for the doubled lattice and the corresponding recursion relations for the parameters. Upon repeating this procedure, the lattice of spacing 2^r is reached with the corresponding, form-conserving equation of motion. After this decimation procedure is performed, the question arises how to obtain the necessary information from it. Studying the problem of superconductive networks [6] it was observed that both the on-site and the off-site coefficients showed a characteristic behaviour as a function of iteration. This was sufficient to distinguish extended solutions from localized ones and regions without solutions. Furthermore it was observed [1] that the behaviour of the on-site coefficient at a certain suitable iteration could give information of the density of states of the problem. This was numerically verified in Ref. [1] on the following models: a) one diagonal impurity in the 1-d, one band, tight-binding model; b) electrons with a site dependent modulating potential: $\varepsilon_n = V_o (\cos Qn + V_1 \cos 2Qn)$ with V_o, V_1 = constants, Q the lattice wave-vector and n the position (this model is quite rich and was studied in some detail by Soukoulis and Economou using different methods [2]).

In all these problems mentioned above [1], [6] the decimation technique had the advantage of requiring much less numerical work than other possible methods. For this reason it is interesting to try it on a model where random

disorder is present. In addition we want to emphasize the advantage of our method over other methods used in disordered systems which in general are approximations (when configurational averages are introduced). In particular we want to compare our results with those obtained by Gonçalves da Silva and Koiller [7] (whose method is also based on the real-space renormalization approach and will be discused below) and those of Southern et al. [8] (who modify Gonçalves da Silva's method in order to overcome its shortcomings without completely succeeding).

For that reason we apply our procedure to disordered binary harmonic chains. We start with the equation of motion for the displacements of the masses from their equilibrium positions:

$$m_i \ddot{u}_i(t) = k \left(u_{i+1}(t) + u_{i-1}(t) - 2 u_i(t) \right) \quad . \tag{1}$$

For a binary system we define $m_i = (n_i)^{-1} m_o$ where $n_i = 1$ with probability p_o and a with probability p_a ($p_o + p_a = 1$). Taking $\omega_o^2 = k / m_o$ the equation of motion reads:

$$(\omega^2 / \omega_o^2 - 2 n_i) u_i + n_i u_{i+1} + n_i u_{i-1} = 0. \tag{2}$$

This can be rewritten as:

$$a_i u_i + n_i^+ u_{i+1} + n_i^- u_{i-1} = 0 \tag{3}$$

where the meaning of a_i is given above, $n_i^{+(-)}$ means the off-diagonal coefficient to the right (left) which become different when decimation is performed. The recursion relations are:

$$\begin{aligned} a_i^{(r+1)} &= \left(a_i - n_{i+k}^- \; n_i^+ / a_{i+k} - n_{i-k}^+ \; n_i^- / a_{i-k} \right)^{(r)} \\ n_i^{+(-)(r+1)} &= - \left(n_{i+k}^{+(-)} \; n_i^{+(-)} / a_{i+k} \right)^{(r)} \end{aligned} \tag{4}$$

where r is the order of iteration and $k = 2^r$. In our method, the on-site coefficient a_i goes to a constant upon iteration and the off-site coefficients $n_i^{+(-)}$ go to zero for ω^2 at which no states are present; both a_i and $n_i^{+(-)}$ go to zero for ω^2 at which localized states exist and both oscillate when extended states appear. Therefore finding all the

possible zeroes of a_i at the iteration when saturation is achieved, in the interval $0 < \omega^2 < 4 \omega_o^2$ gives the necessary information about the density of states. The numerical work required is not much, as detailed below and no approximations such as configurational averages are involved (we just collect all the zeroes coming from a sufficient number of configurations).

Gonçalves da Silva and Koiller [7] start with the equation of motion for the Green's functions which is in some sense similar to eq. (2) with the only difference that it is not equal to zero but to another parameter [8] whose recursion relation has also to be obtained and which is the weight of the pole in the Green's function. The decimation procedure on the equations of motion is performed in the same way as in our method, and due to the fact that the coefficients converge rapidly upon iteration, local Green's functions are obtained. The density of states is extracted from the usual relation ($N(\omega) = -1 / \pi \; \mathrm{Im} \; G_{oo}(\omega + i \, o)$) but this means that they have to use complex frequencies with small imaginary parts whereas we always work with real numbers. For a disordered problem they perform a decimation procedure once and then introduce average values for the parameters. As a consequence they do not obtain gaps, as predicted theoretically for binary disordered chains [9] and as pointed out in Ref. [8] . The authors of Ref.[8] try to improve that method performing the average at a further step of iteration without completely succeeding; the gaps are not present with this type of approach (we think that although small but finite imaginary parts transform localized states in narrow bands which overlap). They also suggest the necessity of performing decimation not on a singular site but on a cluster because certain peaks do not appear with the method of Ref.[7]. We do find those peaks with our procedure (as explained below). As decimation is exact in our approach it should give the same results performed on single site or on clusters or in any other way.

In Fig. 1 the full line corresponds to the pure chain density of states ($N(\omega^2) = \mathrm{const} \; (4 - (\omega^2 / \omega_o^2 - 2)^2)^{-1/2}$. The points are the inverse of the separation of the zeroes of the on-site coefficients at iteration 6 which is the method we have previously presented [1] for the calculation of the density of states. The agreement is very good. The constant adjusts the minimum value of our procedure with the theoretical relation. In Figs.2a) and b) we have collected the zeroes of the on-site coefficient from 10 different configurations (with $a = 3$ and $p_a = .5$). We have worked with iteration 11 for which saturation was obtained, except

at very small ω^2 / ω_o^2 . In a) we plot the zeroes with the height corresponding to the inverse of the separation between them. In b) we form the usual histogram by counting the number of zeroes (states) in a given ω^2 interval. This should be compared with computer simulation results [10] (see Fig. 1, in Ref.[8]). The agreement is good taking into account the small number of configurations analyzed here. No states appear in the forbidden regions as in the Gonçalves da Silva [7] and Southern [8] procedures. In Fig. 3 we make the same analysis for $a = 10000$ and $p_a = .5$. The peak at central frequencies appears in several configurations in our procedure and the modifications suggested by Southern et al. [8] are not necessary to obtain it.

In conclusion we think that the RG decimation technique is a very suitable procedure because convergence is obtained quickly and clear distinction between gaps, localized and extended states exists [1], [6]. In 1-d problems it is exact, even if interactions further than nearest neighbour are present, as was shown recently by Southern et al.[11] . As far as we know for higher dimensions the technique can be applied only with additional approximations because the form is not conserved upon iteration (with each step new couplings appear). This subject is still of current interest [11]. We think that our procedure is superior to that of Gonçalves da Silva et al. [7] because the numerical work is done with real numbers. We have shown here and in a previous paper [1] that the density of states can be obtained without having to go through the theory of Green's functions. In addition, in our procedure the spatial dependence of the wave vectors is obtained directly [1]. For random problems our procedure gives much better agreement with theoretical predictions and numerical simulation data.

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References

[1] C. Wiecko and E. Roman, ICTP , Trieste, preprint IC/83/162. (submitted for publication).

[2] C. M. Soukoulis and E. N. Economou, Phys. Rev. Lett. 48, 1043 (1982).

[3] D. R. Hofstadter, Phys. Rev. B 14, 2239 (1976).

[4] J. B. Sokoloff and J. V. José, Phys. Rev. Lett. 49, 334 (1982).

[5] P. G. de Gennes, C. R. Acad. Sci. Ser.II 292, 9 (1981); 292, 279 (1981).
S. Alexander, Phys. Rev. B 27, 1541 (1983).
H. J. Fink, A. López and R. Maynard, Phys. Rev. B 26, 5237 (1982).

[6] J. M. Simonin, C. Wiecko and A. López, Phys. Rev. B, to be published.

[7] C. E. T. Gonçalves da Silva and B. Koiller, Solid State Commun., 40, 215 (1981).

[8] J. M. Langlois, A. M. S. Tremblay and B. W. Southern, Phys. Rev. B 28, 218 (1983).

[9] H. Watsuda, Prog. Theor. Phys. 19, 161 (1964).
J. Hori, ibid. 31, 940 (1964).

[10] D. N. Payton III and W. M. Visscher, Phys. Rev. 154, 802 (1967).

[11] B. W. Southern, A. A. Kumar, P. D. Loly and A. M. S. Tremblay, Phys. Rev. B 27, 1405 (1983).
B. W. Southern, A. A. Kumar and J. A. Ashraff, Phys. Rev. B 28, 1785 (1983).

Figure Captions

Fig. 1 Full line: the density of squared frequencies for the pure chain ($N(\omega^2) = \text{const} \left(4 - \left(\omega^2 / \omega_o^2 - 2 \right)^2 \right)^{-1/2}$). The points are the inverse of the separation between zeroes of the on-site coefficient at iteration 6.

Fig. 2 The density of states for a random binary chain with $m_1 = m_o/3$ and $p_o = .5$; a) the inverse of the separation between zeroes of the on-site coefficient at iteration 11, b) histogram of those zeroes (states).

Fig. 3 The same as in Fig. 2 for $m_1 = m_o / 10000$ and $p_o = .5$.

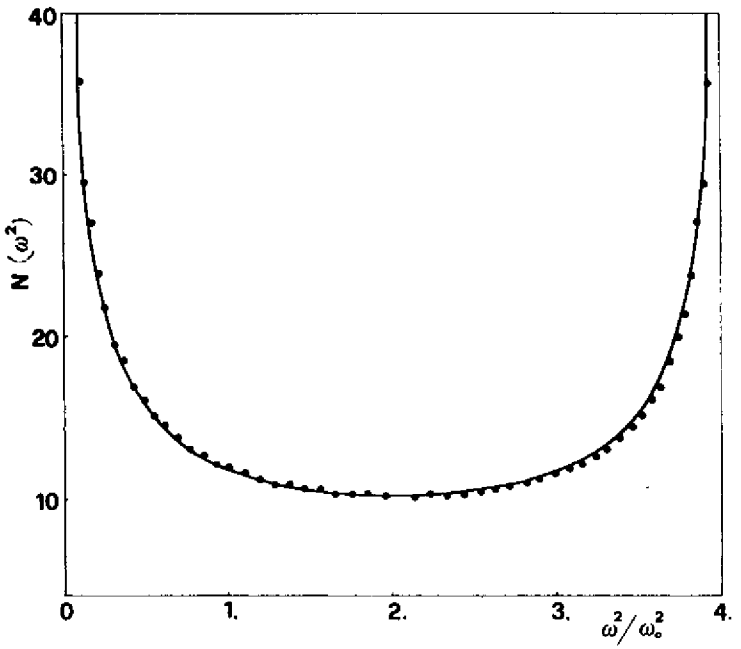

Fig. 1

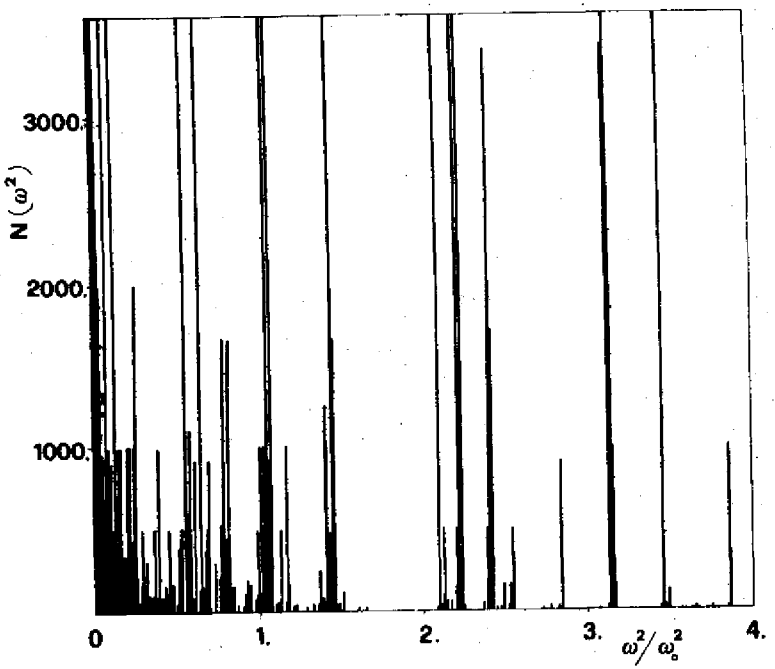

Fig.2 a

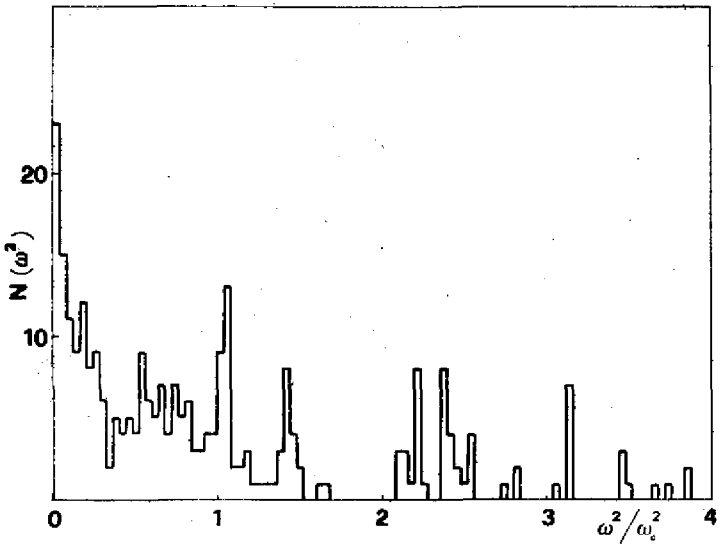

Fig. 2 b

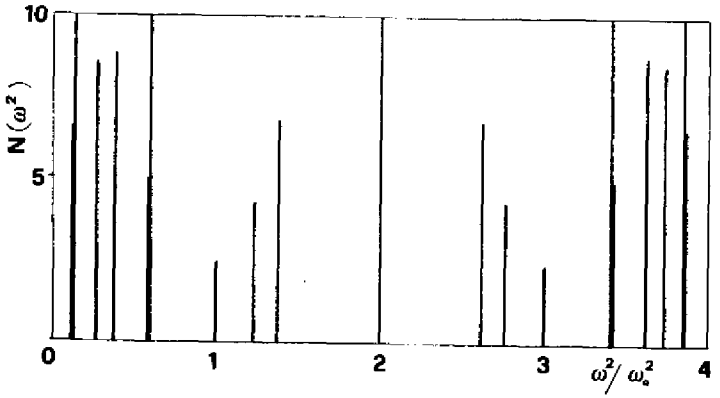

Fig. 3 a

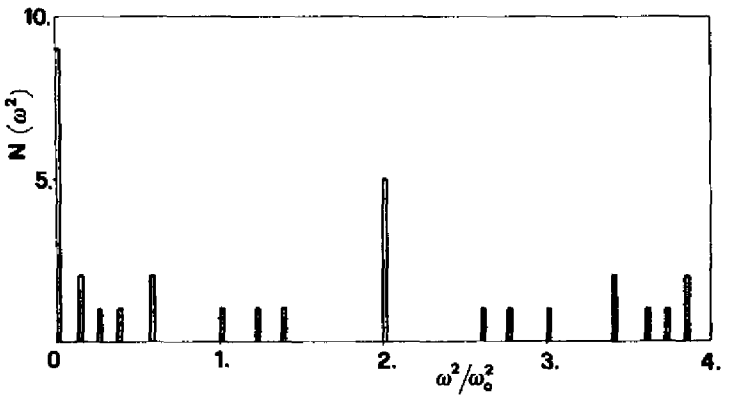

Fig. 3 b