BAND-SPLITTING AND WAVE FUNCTION SCALING IN QUASICRYSTALLINE STRUCTURES

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ABSTRACT: Here we briefly review a renormalization group theory derived from a real space decimation technique. A new result regarding the wave function scaling is presented, and some applications are discussed.

The spectral and wave function properties of one-dimensional quasicrystalline lattices have been extensively studied in recent years. While most work has been done numerically, analytical approaches based on trace maps[1] and real space decimation techniques[2] have played the central role in our understanding of such systems. In 1986, we proposed a renormalization group (RG) theory based on a decimation scheme derived from degenerate perturbation calculations.[2] While it is exact only in a certain limit, it offers us a simple and intuitive picture about the physics of the system. Here we give a brief review of our work and the applications of this RG made by others

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later on. A new result on the wave function scaling will also be mentioned.

The basic idea of our RG theory is quite simple. Consider a tight-binding lattice with constant site energies, and nearest-neighbor (nn) hopping amplitudes $\{T_w, T_s\}$ arranged in a Fibonacci sequence (Figure 1a). We assume $|T_w/T_s| \ll 1$. In the first step of the RG, we diagonalize the strong bonds. If the weak bonds are ignored, then the spectrum will consist of three degenerate levels, corresponding to states on the isolated sites (atoms) and the bonding or anti-bonding states on the pairs of sites (molecules) originally connected by the strong bonds. These levels are separated by the energy $|T_s|$, which is, by assumption, much larger than the ignored weak bonds. When the leading corrections of the weak bonds are taken into account, the different states in a degenerate level are connected, but the states belonging to different levels are decoupled. The result is three independent sub-lattices: 1) bonding molecular chain, 2) atomic chain and 3) anti-bonding chain. They have renormalized nearest-neighbor bonds

$$\{\, T_w^2/2T_s,\ T_w/2 \,\}\ ,\ \{\, T_w^3/T_s^2,\ -T_w^2/T_s \}\ ,\ \{\, T_w^2/2T_s,\ -T_w/2 \},$$

respectively, all arranged in a Fibonacci sequence as $\{T_w, T_s\}$ was in the original lattice. In the subsequent steps of the RG, each of the sublattices are renormalized again into three sub-sublattices, and so on.

A direct consequence of this RG analysis is that the spectrum should have a hierarchical pattern: three major clusters, each of which is trifurcated into three subclusters, and so on. The middle subclusters correspond to the atomic sublattices, and they are narrower by a factor of $|T_w/T_s|$ than the side subclusters sharing the same parent cluster. The relative spectral weights of the three subclusters from a given parent cluster is

$$\left(\frac{1}{\tau^2},\ \frac{1}{\tau^3},\ \frac{1}{\tau^2}\right),$$

as can be obtained by counting the relative number of sites involved in a sublattice.

These results have provided a simple analytic basis for a global scaling analysis of the spectrum by Zheng.[3] His result compares qualitatively well with the numerical result of ref. 1 and is exact in the limit of $|T_w/T_s| \ll 1$.

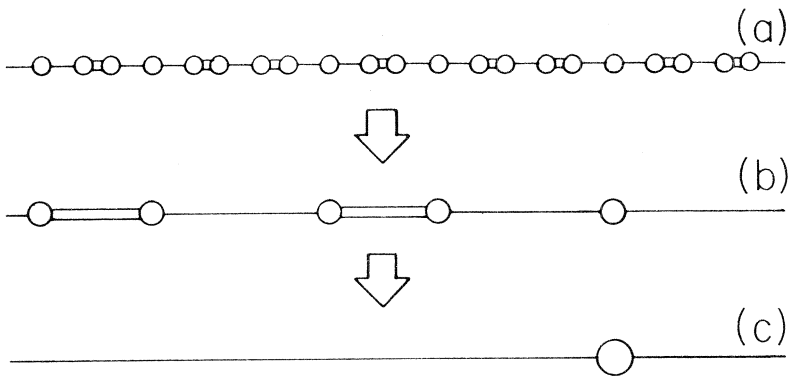
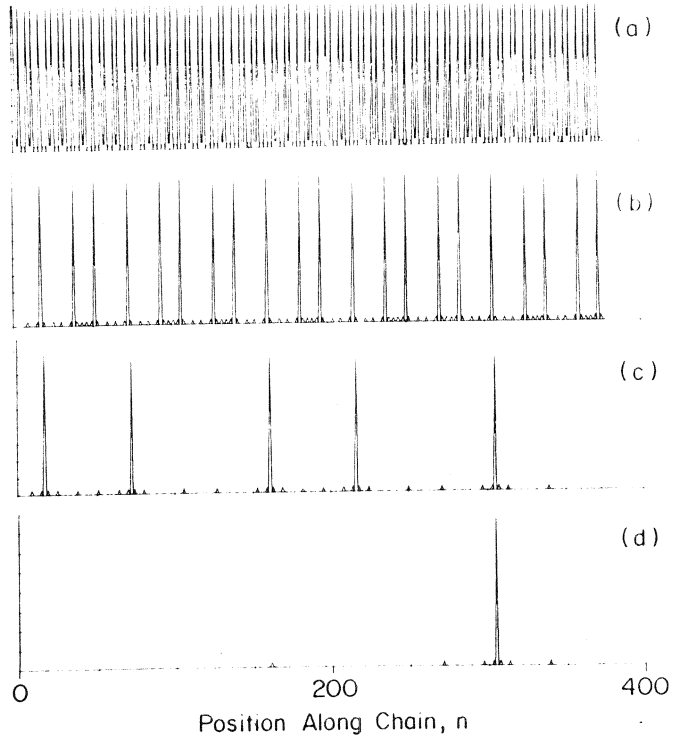


Figure 1: Schematic representation of the renormalization–group decimation technique for the central subbands ("atomic-type") of the energy spectrum of a tight-binding Fibonacci lattice. This decimation procedure favors the atomic (i.e., weakly coupled or isolated) sites and is useful in order to study the central part of the nth-furcation of the spectra. The double lines denote the strong effective bonds, i.e. large overlap integrals or hopping amplitudes. The single lines represent the weak effective bonds. The atoms in (a) are represented by open circles. The strongest bonds between atoms form bound states (molecules). The molecules in (a) are eliminated, producing the renormalized chain in (b). The larger circles represent the new (renormalized) atoms. Again, the short distances between the atoms correspond to the strong bonds (double lines) which define the new molecules of the chain. Eliminating the new molecules, we obtain the renormalized chain in (c), where the only circle represents the new renormalized isolated site.

Figure 2: Probability density, $P_n = \sum_s |\psi_n^{(s)}|^2$ summed over the states belonging to a given cluster, versus site position, n, along the chain. In (a)–(d) the probability densities have contributions from the states belonging respectively to (a')–(d'), where (a') denotes the central main cluster of states around $E = 0$ in the energy spectra, (b') the central subcluster of (a'), (c') the central subcluster of (b'), and (d') the central subcluster of (c'). It is important to note that the lattices of figures 1(a), 1(b), and 1(c) correspond to the probability densities (b), (c), and (d) respectively.



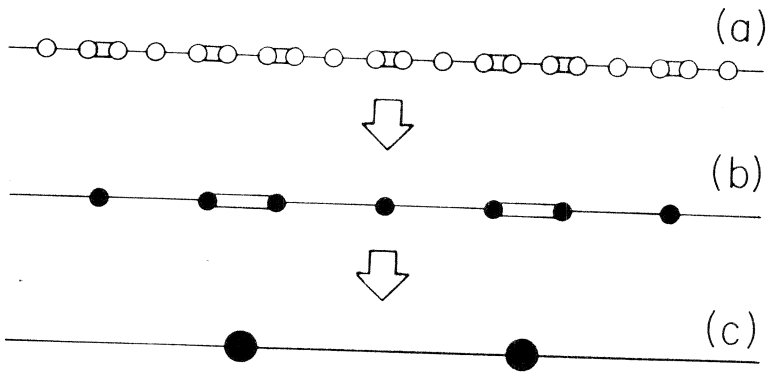


Figure 3: Schematic representation of the decimation procedure f avoring the bonding (i.e., strongly coupled) molecular states. This procedure is useful in order to study the edge states of the nth-furcation of the spectra. The double (single) lines denote the strong (weak) effective bonds. The atoms are represented by open circles. The strong bonds between atoms form bound states (molecules). The weakly coupled atoms in (a) are decimated, producing the renormalized chain in (b). The black circles represent the new weakly–coupled sites. Eliminating these isolated atoms we obtain the renormalized chain in (c), where the larger black dots represent the new atoms (molecules according to the lattice (b), and supermolecule – or cluster of molecules – according to (a)).

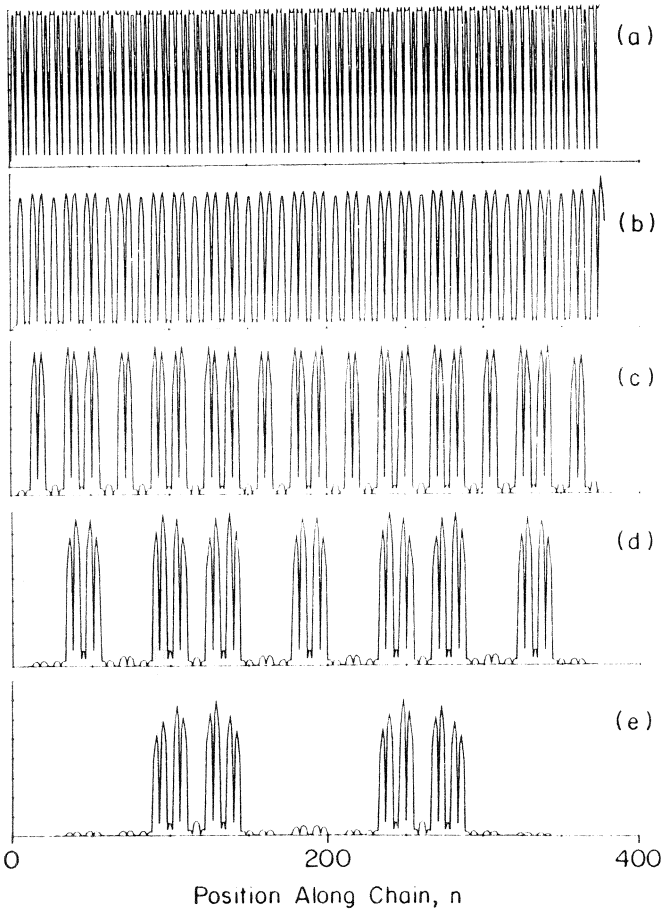


Figure 4: Probability density, P_n, versus site position, n , along the chain. In (a)–(e) the probability densities have contributions from the states belonging respectively to (a")–(e"), where (a") denotes the top main cluster of states in the energy spectra, (b") the top subcluster of (a"), (c") the top subcluster of (b"), and so on. It is remarkable to note that the lattices of figures 3(a), 3(b), and 3(c) correspond to the probability densities of (c), (d), and (e) respectively.

Another consequence of the RG analysis is that certain wave functions ıcale with distances. Consider the state with an energy in the center of the ıpectrum. This state is coded by the symbolic string *cccc*...., meaning that he energy belongs to the central cluster, the central subcluster of the central :luster, and so on. According to the RG analysis, in each step of specializing nto a sublattice, the wave function gets enhanced by a factor of $|T_s/T_w|$, vhile the average distance between the sites, L, gets enlarged by a factor of 3. We therefore have

$$|\psi(L)| \sim L^{\ln|T_s/T_w|/\ln 3}$$

vhere L is a distance along the chain. Next we consider a state at the edge of he spectrum. This state is coded as *sss*..., meaning that the energy belongs o the side cluster, a side subcluster of side cluster, and so on. In this case, he average distance between sites gets enlarged by a factor of 2 by enormalization. Therefore

$$|\psi(L)| \sim L^{\ln|T_s/T_w|/\ln 2}.$$

'hese results have also been obtained[1] using trace map formulas. Finally, 'e consider a state coded by a string of mixed s and c's. If the concentration f the c's is ρ_c and that of the s's is ρ_s, then we should have

$$|\psi(L)| \sim L^{\ln|T_s/T_w|/\ln 3^{(2\rho_s+3\rho_c)}}.$$

his is, up to our knowledge, a new result.

Our RG theory has also been applied to an analysis of the roughening two-dimensional quasicrystal interfaces by Garg[4]. In particular, he com- ıtes the leading low-temperature behavior of the roughness exponent. In ı appendix of his article, he obtains, and also rederives in slightly different ırms, some basic results of the RG theory.

Finally, we should mention that our RG theory can be very naturally ›plied to lattices with hierarchical couplings.[5]

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