

Review



Real Space Theory for Electron and Phonon Transport in Aperiodic Lattices via Renormalization

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Received: 7 February 2020; Accepted: 3 March 2020; Published: 7 March 2020



Abstract: Structural defects are inherent in solids at a finite temperature, because they diminish free energies by growing entropy. The arrangement of these defects may display long-range orders, as occurring in quasicrystals, whose hidden structural symmetry could greatly modify the transport of excitations. Moreover, the presence of such defects breaks the translational symmetry and collapses the reciprocal lattice, which has been a standard technique in solid-state physics. An alternative to address such a structural disorder is the real space theory. Nonetheless, solving 10²³ coupled Schrödinger equations requires unavailable yottabytes (YB) of memory just for recording the atomic positions. In contrast, the real-space renormalization method (RSRM) uses an iterative procedure with a small number of effective sites in each step, and exponentially lessens the degrees of freedom, but keeps their participation in the final results. In this article, we review aperiodic atomic arrangements with hierarchical symmetry investigated by means of RSRM, as well as their consequences in measurable physical properties, such as electrical and thermal conductivities.

Keywords: quasiperiodicity; localization; tight-binding model; Kubo formula; low-dimensional systems

1. Introduction

Nowadays, impurities and defects in solids play a central role in microelectronics and modern materials science, because they deeply alter the propagation and interference of electronic wave functions [1]. In general, structural disorder obstructs the transport of excitations. However, this obstruction to both electronic and phononic transport could become beneficial, such as for the thermoelectricity, whose figure of merit is a function of the ratio between electrical and thermal conductivities [2].

Since the formulation of quantum mechanics at the beginning of the last century, the study of crystalline solids is carried out through the reciprocal lattice and local imperfections are addressed as perturbations [3]. For extended random disorders, the coherent potential approximation (CPA) is used in their analysis [4]. The discovery of quasicrystals by D. Shechtman et al. in 1984 [5] has stimulated the development of new techniques to investigate the long range and hierarchically located impurities or defects. During many years, the quasiperiodic systems have been studied using approximants [6], whose artificial periodic boundary condition has deep effects on the entire band structure of a truly quasiperiodic lattice, as illustrated in Figure 1.

To address macroscopic aperiodic lattices, the traditional reciprocal space [7] approach becomes inappropriate or useless, as the aperiodicity collapses the first Brillouin zone. An alternative way could be the real-space renormalization method (RSRM) firstly proposed by Leo P. Kadanoff [8] for

condensed matter physics in 1966, to realize a scaling analysis of magnetization in terms of spin blocks, which exponentially reduces the degrees of freedom, keeping only the lower energy states. In 1971, Kenneth G. Wilson [9,10] reformulated the RSRM to introduce the universality classes of scale-independent critical points in phase transitions and was awarded by the Nobel Prize in Physics for this work in 1982.



Figure 1. (color online) (**a**,**b**) Density of states (DOS) and (**c**,**d**) zero-temperature direct current (DC) conductivity (σ) versus the chemical potential (μ) for two bond-disordered Fibonacci chains (**b**,**d**) of n = 57 and (**a**,**c**) with a unit cell of n = 15. Insets (**a**'-**d**') are the respective magnifications of (**a**-**d**) spectra.

In this article, we first introduce the tight-binding model and the Kubo–Greenwood formula [11] to describe the electronic transport in Fibonacci chains, as well as RSRM developed to reach macroscopic length. Other aperiodic chains, beyond the quasiperiodic ones, are further presented with a special emphasis on their electronic wave-function localization and the ballistic transport states. Studies on multidimensional aperiodic lattices are subsequently summarized, where the combination of RSRM with convolution theorem is shown. In Section 5, we discuss vibrational excitations or phonons in aperiodic lattices, as well as the thermoelectric transport in segmented heterostructures. Final remarks will be given in the conclusion section.

2. Fibonacci Chains

Let us first consider a single electron in a periodic lattice of atoms, which is usually addressed by means of Bloch's theorem [3]. This theorem establishes a general solution of the Schrödinger equation for a periodic potential, and then the electronic wave functions are commonly written as a linear combination of plane waves. Alternatively, such wave functions can also be expressed in terms of atomic orbitals, because they constitute another base for solutions of the Schrödinger equation. In fact, the orthonormalized orbitals of all atoms, known as Wannier functions, are the Fourier transformed Bloch functions [3].

For aperiodic lattices, the Wannier functions localized at each atom remain as a useful base. The single-band electronic Hamiltonian within the tight-binding formalism can be written as

$$H = \sum_{j} \varepsilon_{j} |j\rangle \langle j| + \sum_{\langle j,l \rangle} t_{j,l} |j\rangle \langle l|$$
(1)

where ε_j is the self-energy of atom j with Wannier function $|j\rangle$ and $t_{j,l}$ is the hopping integral between the nearest-neighbor atoms j and l denoted by $\langle j, l \rangle$. The density of states (DOS) can be calculated using the single-electron Green's function (*G*) [12]:

$$DOS(E) = -\frac{1}{\pi} \lim_{\eta \to 0^+} \operatorname{Im} Tr[G(E + i\eta)]$$
⁽²⁾

where η is the imaginary part of energy *E* and the Green's function is determined by the Dyson equation given by (E - H)G = 1.

Within the linear response theory, the electrical conductivity (σ) can be determined by means of the Kubo–Greenwood formula [11,12]:

$$\sigma_{xx}(\mu,\omega,T) = \frac{2e^2\hbar}{\Omega\pi m^2} \int_{-\infty}^{\infty} dE \frac{f(E) - f(E + \hbar\omega)}{\hbar\omega} Tr \Big[p_x \text{Im}G^+(E + \hbar\omega) p_x \text{Im}G^+(E) \Big]$$
(3)

where Ω is the system volume, $p_x = (im/\hbar)[H, x] = (ima/\hbar)\sum_j \{t_{j,j+1}|j\rangle\langle j+1|-t_{j,j-1}|j\rangle\langle j-1|\}$ is the projection of the momentum operator along the applied electrical field with $x = \sum_j ja|j\rangle\langle j|$, $G^+(E) = G(E + i\eta)$ is the retarded Green's function, and $f(E) = \{1 + \exp[(E - \mu)/k_BT]\}^{-1}$ is the Fermi–Dirac distribution with the chemical potential μ and temperature *T*. The electrical conductivity of direct current (DC) at zero temperature of a periodic linear chain ($t_{j,l} = t$) of *N* atoms with null self-energies is as follows [13]:

$$\sigma_P = \sigma(\mu, 0, 0) = \frac{(N-1)ae^2}{\pi\hbar}$$
(4)

when the chemical potential is found in the allowed energy band, that is, $|\mu| \le 2|t|$. It would be worth mentioning that the non-uniformity of atomic locations can be introduced through replacing the hopping integrals $t_{j,l}$ by $\tilde{t}_{j,l} = |x_j - x_l| t_{j,l} / a$ in the momentum operator expression.

The most studied quasiperiodic system is the Fibonacci chain, shown in Figure 2a, which can be built using two sorts of bonds (bond problem), two kinds of atoms (site problem), or a combination of both (mixing problem) [14]. For example, in the bond problem, the nature of atoms is assumed to be the same ($\varepsilon_j = 0$) and two bond strengths t_A and t_B are ordered following the Fibonacci sequence [15,16], whose atomic chain of generation *n* can be obtained using the concatenation of two previous generations, $F_n = F_{n-1} \oplus F_{n-2}$, with the initial conditions of $F_1 = A$ and $F_2 = AB$.

In Figure 1, we present (a,b) the density of states (DOS) and (c,d) the DC electrical conductivity at zero temperature (σ) as functions of the chemical potential (μ) for (a,c) a Fibonacci chain with bond disorder of $t_A = \frac{1}{2}(\sqrt{5}-1)t$ and $t_B = t$ made of a unit cell of generation n = 15 (987 bonds) repeated by $2^{29} = 536,870,912$ times, resulting a chain of N = 529,891,590,145 atoms connected to two leads built by repeating 2^{100} times the mentioned unit cell, and (b,d) a Fibonacci chain of generation n = 57 with N = 591,286,729,880 atoms having the same bond disorder strength as in (a,c). Both DOS and σ results were calculated by means of the renormalization method developed in [17] with grids of (a–d) 800,000 and (a'–d') 300,000 data. The imaginary parts of energy used in these figures are $\eta = 10^{-6}|t|$ for DOS and $\eta = 10^{-14}|t|$ for σ spectra.



Figure 2. (color online) Schematic representations of one-dimensional (a) Fibonacci, (b) Thue-Morse, (c) branched, and (d) molecular chains, as well as two-dimensional (e) Penrose, (f) Fibonacci, (g) labyrinth, and (h) Poly(G)-Poly(C) lattices.

Observe the close similarity between *DOS* spectra shown in Figure 1a,b in contrast to the conductivity spectra of Figure 1c,d, as well as the remarkable differences between Figure 1a', b', where the continuum energy bands in Figure 1a' are originated from the periodic repetition of a unit cell. These differences can significantly modify the calculation of many physical quantities weighted by DOS spectra, such as the specific heat, optical absorption, and low-temperature DC and alternating current (AC) conductivities. Hence, the accurate determination of DOS and σ spectra constitutes a crucial starting point for the study of quasiperiodic systems.

The RSRM has been applied to quasiperiodic systems described by tight-binding Hamiltonian (1) since the discovery of quasicrystals. For example, from 1984 to 1987, M. Kohmoto and collaborators carried out renormalization group studies of Cantor-set electronic band spectra [18,19], the diffusion coefficient [20], localization properties [21,22], and the resistance power–law growth with sample length [23]. Q. Niu and F. Nori developed, in 1986, a decimation procedure to calculate energy spectra of Fibonacci chains based on the weak bond approximation [24], which was also applied to a scaling analysis of sub-band widths [25]. In 1988, H. E. Roman derived a RSRM to calculate on-site energies and hopping integrals of each generation [26], P. Villaseñor-González, F. Mejía-Lira, and J. L. Morán-López calculated the electronic density of states in off-diagonal Fibonacci chains [27], while C. Wang and R. A. Barrio obtained [28] the Raman spectrum measured in GaAs-AlAs quasiperiodic superlattices [29]. Moreover, the RSRM has also been used for the local electronic density of states [30],

Ising model [31,32], and alternating current (AC) conductivity [33] through the resistance network model of Miller and Abrahams [34].

In the 1990s, more attempts were registered to develop and use the renormalization technique. For example, J. C. López, G. G. Naumis, and J. L. Aragón determined [35] the electronic band structure of disordered Fibonacci chains following the renormalization procedure of Barrio and Wang [36]; while R. B. Capaz, B. Koiller, and S. L. A. de Queiroz studied the power–law localization behavior [37]; Y. Liu and W. Sritrakool found energy spectrum branching rules [38]; A. Chakrabarti et al. analyzed the nature of eigenstates [39]; and J. X. Zhong et al. calculated the local [40] and average [41] density of states. Besides, AC conductivity was examined [42,43] within the Miller and Abrahams approach. During the second half of the decade, F. Piéchon, M. Benakli, and A. Jagannathan established analytical scaling properties of energy spectra [44]; E. Maciá and F. Domínguez-Adame proved the existence of transparent states [45]; while A. Ghosh and S. N. Karmakar explored the second-neighbor hopping problem [46].

From the twenty-first century, the electronic transport in Fibonacci chains was deeply studied via renormalization. For instance, V. Sánchez et al. developed, in 2001, a sophisticated and exact RSRM for the Kubo–Greenwood formula (3) applied to the mixing Fibonacci problem [47], and then its AC conductivity spectra were carefully analyzed [48,49] beyond those obtained from approximants [50]. The renormalization technique was also used for the study of localization [51–53], electronic spectra of GaAs/Ga_xAl_{1-x}As superlattices [54], and arrays of quantum dot [55], as well as for a unified transport theory of phonon [56], photon [57], and fermionic atom [58] based on the tight-binding model. On the other hand, by means of RSRM, the fine structure of energy spectra [59] and electronic transport in Hubbard Fibonacci chains [60,61] were investigated, and a new universality class was found in spin-one-half Heisenberg quasiperiodic chains [62].

3. Aperiodic Chains besides Fibonacci

Among aperiodic sequences, the generalized Fibonacci (GF) order was one of the most studied, which can be obtained by the substitutional rule:

$$A \to A^{u}B^{v} \operatorname{?and} B \to A \tag{5}$$

or using the substitution matrix (**M**):

$$\begin{pmatrix} A \\ B \end{pmatrix} \to \mathbf{M} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} u & v \\ 1 & 0 \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} \underbrace{AA \cdots ABB \cdots B}_{u} \\ \underbrace{u} & v \\ A \end{pmatrix}$$
(6)

where *u* and *v* are positive integer numbers. Matrix **M** has the following eigenvalues (λ_{\pm}):

$$\begin{vmatrix} u - \lambda & v \\ 1 & -\lambda \end{vmatrix} = 0 \implies \lambda^2 - u\lambda - v = 0 \implies \lambda_{\pm} = \frac{u \pm \sqrt{u^2 + 4v}}{2}$$
(7)

For v = 1, Equation (7) leads to $\lambda_+ > 1$ and $|\lambda_-| < 1$, which fulfill the Pisot conjecture [14,63]. Moreover, the determinant of **M**,

$$\det(\mathbf{M}) = \begin{vmatrix} u & v \\ 1 & 0 \end{vmatrix} = -v \tag{8}$$

is unimodular if v = 1. Hence, the corresponding sequences are called quasiperiodic and possess Bragg-peak diffraction spectra, because both the Pisot eigenvalue condition and the unit-determinant requirement of **M** are satisfied [64]. On the contrary, the GF sequences with $v \neq 1$ do not satisfy the unit-determinant requirement and thus they are not quasiperiodic. When u = v = 1, the sequence is called golden mean or the standard Fibonacci one, while the cases u = 2 and u = 3 are named silver and bronze means, respectively, when v = 1, which are also known as the precious means. In addition, the metallic means stand for the sequences with u = 1 and v > 1 [65].

Since 1988, the electronic properties of GF chains have been investigated [66] and the RSRM was applied for calculating the average Green's function [67,68], local [69–73], and integrated [74,75] density of states, as well as for analyzing the localization of eigenstates [76]. Nonequilibrium phase transitions were analyzed by means of RSRM and Monte Carlo approaches [77]. Recently, the ballistic transport was found at the center of energy spectra in macroscopic GF chains with bond disorder every six generations when v = 1 or all generations when u and v are both even numbers [78], whose wave-function localization and electrical conductivities (DC and AC) were investigated through a system length scaling analysis [79].

On the other hand, the Thue–Morse (TM) sequence constitutes another widely studied aperiodic order, whose nth generation chain, denoted by TM_n , can be constructed using the substitution rule $A \rightarrow AB$ and $B \rightarrow BA$, or the addition rule $TM_n = TM_{n-1} \oplus \overline{TM_{n-1}}$, where the symbol \oplus stands the string concatenation and $\overline{TM_n}$ is the complement of TM_n , obtained by exchanging A and B in TM chains. The initial condition is $TM_0 = A$, and thus $TM_3 = ABBABAAB$ has 2^3 atoms, being the eight most left atoms in Figure 2b. The TM sequence accomplishes the Pisot conjecture, but it has a null substitution matrix determinant, det(\mathbf{M}) = 0, as periodic lattices [80]. In consequence, it is not a quasiperiodic system, but exhibits an essentially discrete diffraction pattern, and then TM heterostructures can be regarded as an aperiodic crystal according to the definition of crystals given by the International Union of Crystallography [81]. The RSRM has been applied to the study of electronic properties in TM chains since 1990 [82], where the density of states [83], trace map problem [84,85], and localization [86,87], as well as excitonic states [88], were analyzed.

Another example of aperiodic sequence studied by RSRM was period doubling (PD), whose sequence can be generated by substitutions $A \rightarrow AB$ and $B \rightarrow AA$, or the addition rule $PD_n = PD_{n-1} \oplus PD_{n-2} \oplus PD_{n-2}$, where PD_n is the PD chain of generation n and the initial conditions are $PD_0 = A$ and $PD_1 = AB$. For example, $PD_2 = ABAA$ and $PD_3 = ABAAABAB$. The local [89] and global [90] electronic properties of pristine and random PD chains, as well as critical behavior of the Gaussian model [91], were studied via RSRM. Moreover, three-component Fibonacci chains, defined by the inflation rules $A \rightarrow B$, $B \rightarrow C$, and $C \rightarrow CA$, were addressed by the RSRM, where branching rules of their electronic energy spectra were analytically obtained [92] and compared with the numerical local density of states [93]. A summary on the nature of electronic wave functions in one-dimensional (1D) aperiodic lattices can be found in [94].

4. Multidimensional Aperiodic Lattices

Beyond one-dimensional systems, let us first consider a linear chain with branches of atoms, known as Fano-Anderson defects [95], which is illustrated in Figure 2c and has an average coordination number of larger than two, but without loops. The appearance of such branches may significantly modify the transport of excitations along the linear chain owing to the wave interference. In fact, quasiperiodically placed branches could inhibit the transport of long-wavelength excitations, which are usually unaltered by local impurities or defects [96]. Electronic transport in a quantum wire with an attached quantum-dot array was studied by P. A. Orellana et al. in 2003 [97], while engineering Fano resonances in discrete arrays were proposed by A. E. Miroshnichenko and Y. S. Kivshar in 2005 [98]. During the next decade, more detailed studies using RSRM were carried out for the transmission coefficient [99–105], Landauer resistance [106], Lyapunov exponent [100], local DOS [101–103], and Kubo conductivity [107]. Moreover, the ballistic AC conductivity of periodic lattices has been surpassed through quasiperiodicity [108] or Fano resonances [109].

Linear chains built by ring molecules, illustrated in Figure 2d, constitute another example of systems with an effective dimensionality bigger than one, whose atomic loops produce a rich quantum interference of the conducting wavefunction. This interference enables high-performance molecular switching with large on/off ratios essential for the next generation of molecular electronics [110,111],

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where the RSRM has been used for the study of Fibonacci arrays of Aharonov–Bohm rings [112], metal–insulator transition in the quasiperiodic Aubry model [113], electronic transmission in bent quantum wires [114], and in ladders with a single side-attached impurity [115]. Recently, the electronic density of states, localization, transmittance, and persistent current in molecular chains and ladders have been widely investigated via RSRM [116–122], while the spin-selective electronic transport was also analyzed [123,124]. A review of these studies is presented in [125].

Self-assembled deoxyribonucleic acid (DNA) molecular wires, built by cytosine-guanine (CG) or adenine-thymine (AT) stacked pairs attached to the double-helix structure through sugar-phosphate backbones, may behave as a low-dimensional conductor, semiconductors, or insulators, depending on the system length and base-pair sequences [126,127]. Ab-initio [128,129] and semi-empirical [130,131] studies of DNA molecules were carried out and, among them, the latter has the advantage of being simple and suitable for the analysis of electronic transport in aperiodic double chains with macroscopic length. The DNA molecules can be modelled as a double-strand ladder of coarse grains, which has been transformed into a single string of base pairs with dangling backbones, known as the fishbone model, and in turn, it was reduced to a single chain after a two-step renormalization at each base pair [132]. This chain has been used for the study of electronic transport in Fibonacci [133,134] and asymmetric [135] DNA molecules, helical structures [136–138], thermoelectric devices [139], diluted random base-pair segments [140], and Hubbard systems [141]. An additional renormalization process can be carried out along organic molecular wires to calculate the density of states [142,143], Lyapunov coefficient [144,145], transmittance [142–145], and magnetoconductance [146]. In fact, the double-strand ladder model is still used for the analysis of charge transport in quasiperiodic Poly (CG) systems [147] and a comparison between ladder and fishbone models was also performed [148]. Moreover, a possible test of the Efimov states in three-strand DNA systems was proposed [149,150]. Several review articles about DNA-based nanostructures have recently been published [151,152].

A two-dimensional (2D) square Fibonacci lattice can be constructed by superimposing two 1D Fibonacci chains along the *x* and *y* axis, as shown in Figure 2f, whose Hamiltonian could be defined as $H^{2D} = H_x^{1D} \otimes I_y^{1D} + I_x^{1D} \otimes H_y^{1D}$ with H_v^{1D} (I_v^{1D}) the 1D Hamiltonian (identity matrix) along the v = x or *y* axis. Hence, for the bond problem, this construction procedure is straightforward [153], while three kinds of sites are generated in the site or mixing problems [154]. A special case of Fibonacci superlattices is obtained when one of these chains is quasiperiodic and another is periodic, in which the 2D problem can be addressed by applying the reciprocal space technique along the periodic direction and the renormalization method along the quasiperiodic one [155]. For the three-dimensional (3D) case, a Fibonacci superlattice is generally obtained from a 2D periodic lattice and a 1D quasiperiodic one, as occurring in the quasiperiodic GaAs-AlAs heterostructure constructed by R. Merlin et al. [156], whose vibrational spectrum was calculated by a combined method of real and reciprocal spaces [28]. In the last three decades, the splitting rules of electronic energy spectra [157–159], density of states [160,161], and DC [162–164] and AC [165,166] electrical conductance in 2D Fibonacci lattices have been extensively studied.

For 3D aperiodic systems with a small cross section, that is, non-periodic nanowires, the electrical conductance [167,168] and impurity effects [169,170] were investigated by means of the renormalization plus convolution technique of [17], whose computational efficiency is shown in Figure 3 and compared to the direct calculation through the matrix inversion process. The computing times shown in Figure 3 correspond to the calculations of zero-temperature DC conductivity given by Equation (3) at $\mu = 0$ for a quasiperiodic nanowire with a cross section of 5×5 atoms, where the Fortran's quadruple precision and a Supermicro workstation with two central processing unit (CPU) processors of Intel Xeon 4108 and 64 GB of DDR4-2666 RAM memory were used. Observe the cubic computing-time increase for the direct calculation case, in contrast to the logarithmic growth when the renormalization plus convolution method is used, which permits the study of electronic transport in truly macroscopic 3D lattices with multiple aperiodically located interfaces. Note also that, for short-length nanowires of 50 atoms, for example, the direct calculation represents a more efficient option than the renormalization one.



Figure 3. (color online) A log–log plot of single-energy Kubo conductivity computing time versus the total number of atoms in a quasiperiodic nanowire with a cross section of 5×5 atoms schematically illustrated in the inset, where the calculations were performed using a Fortran inversion subroutine (blue squares) and the renormalization plus convolution method of [17] (red circles).

Another widely studied 2D quasiperiodic lattice is the Penrose tiling, shown in Figure 2e, whose integrated density of states (IDOS) presents a central peak with about 10% of the total number of states separated from two symmetric bands by two finite gaps [171,172]. The presence of these gaps in macroscopic Penrose lattices has been confirmed by a real-space renormalization study [173] and analyzed by means of a square of the Hamiltonian (H^2) obtained from renormalizing one of the alternating sublattices, because the Penrose tiling is bipartite. The band center of the original Hamiltonian is mapped to the minimum eigenvalue of H^2 , whose eigenfunction has antibonding symmetry and is frustrated by triangular cells in H^2 [174,175]. At the same time, the local [176] and total [177] electronic density of states in Penrose lattices were also studied by a renormalization method, neglecting the small hopping integrals corresponding to the long diagonal of kites. Similar renormalization procedures have been applied to the study of the bond percolation problem [178], phason elasticity [179], Potts spin interaction [180], critical eigenstates [181], and Hubbard model within the real-space dynamical mean-field theory [182,183].

In general, an exact RSRM for 2D Penrose lattices requires the explicit consideration of all boundary sites in each generation to calculate the next-generation Green's function, because it counts all possible paths between two arbitrary sites. This fact inhibits a suitable application of RSRM to truly macroscopic Penrose lattices, in contrast to 1D systems, where the number of boundary sites is always two. Hence, hypercubic aperiodic lattices are commonly addressed by using a renormalization plus convolution method [17].

Labyrinth lattices, shown in Figure 2g, constitute an example of non-cubically structured 2D aperiodic tiling, where a novel convolution plus renormalization method has been successfully applied [184], being the first aperiodic multidimensional lattice beyond hypercubic structures investigated by means of RSRM. This lattice was first introduced by C. Sire in 1989 obtained from a Euclidean product of two 1D aperiodic chains [185,186]. The energy spectrum of the Labyrinth tiling has been proven to be an interval if parameters λ_x and λ_y of the *x* and *y* direction chains, defined

by $\lambda \equiv |t_A^2 - t_B^2|/t_A t_B$, are sufficiently close to zero, and it is a Cantor set of zero Lebesgue measure if λ_x and λ_y are large enough [187,188]. The wave packet dynamics [189] and quantum diffusion [190] in the Labyrinth tiling were also analyzed using RSRM. Labyrinth lattices based on silver-means quasiperiodic chains have been observed in a surface-wave experiment [191].

5. Vibrational Excitations

A solid of N atoms has 3N degrees of freedom and it can translate or rotate as a whole, hence it may have 3N - 6 normal modes of vibration, in which all atoms move sinusoidally with the same frequency and a fixed phase relation [3,192]. The quantum of these normal vibrational modes is called phonon, who has crucial participation in the Raman scattering [193], infrared (IR) spectroscopy [194], and inelastic neutron scattering [195], as well as in thermal transport [196]. These phonons, as other elementary excitations in solids, are scattered by impurities, defects, and structural interfaces, and their transport in quasiperiodic lattices has been studied since the discovery of quasicrystals. For example, the first quasiperiodic GaAs-AlAs superlattice was built in 1985 [156] and its acoustic Raman spectrum measured from the backscattering [29] was theoretically reproduced in 1988 [28]. Using RSRM, the phonon frequencies [197,198], local DOS [199,200], transmission coefficient [201], and lattice specific heat [202] in Fibonacci chains, as well as vibrational properties in Thue–Morse [202,203], period-doubling [204], Rudin–Shapiro [204], and three-component Fibonacci [205] systems, were studied. Experimental determination of phonon behavior was carried out in 1D aperiodic lattices through the third sound on a superfluid helium film [206], while in 2D Penrose tiling using quasiperiodic arrays of Josephson junctions [207], tuning forks [208], and LC electric oscillators [209], in which anharmonic effects were also analyzed.

The lattice thermal conductance (*K*) given by Equation (5) of [210] is calculated using the RSRM and comparatively presented in Figure 4 for periodic (165,580,142 atoms), Fibonacci (165,580,142 atoms), Thue–Morse (134,217,729 atoms), and period doubling (134,217,729 atoms) chains with a uniform mass *M* and restoring force constants $\alpha_A = \frac{1}{2}(\sqrt{5}-1)\alpha$ and $\alpha_B = \alpha$ connected to two periodic leads at their ends, where $K_0 = \pi k_B \omega_0/6$ is the quantum of thermal conductance [211], $\omega_0 = \sqrt{\alpha/M}$, and $T_0 = \hbar \omega_0/k_B$. In general, the thermal conductance of aperiodic chains diminishes with the structural disorder strength and the system length, whose temperature variation K(T) is consistent with those reported in [212]. The corresponding phonon transmittance spectra are shown in Figure 4a for Fibonacci, Figure 4b for period doubling, and Figure 4c for Thue–Morse chains in comparison with that of the periodic one illustrated by the dark-yellow solid lines in each of them, while a low-temperature magnification of K(T) - T is exposed in Figure 4d for the mentioned chains. Observe in Figure 4d the nearly linear behavior of K(T) for the periodic case whose small deviation is caused by the finite length of system, and the presence of a crossing between K(T) curves of Fibonacci and Thue–Morse chains, where the higher K(T) of Thue–Morse chains at low temperature is originated from its almost one transmittance around the zero vibrational frequency, as shown in Figure 4c.



Figure 4. Lattice thermal conductance (K) as a function of temperature (T) for periodic (circles), Fibonacci (squares), period doubling (up triangles), and Thue–Morse (down triangles) chains. Insets: the corresponding phononic transmittance spectra of (**a**) Fibonacci, (**b**) period doubling, and (**c**) Thue–Morse chains, as well as (**d**) an amplification of $K(T)/K_0$ –T at the low-temperature zone.

For 3D systems, the real-space renormalization plus convolution method has been applied to the study of lattice thermal conductivity by phonons in quasiperiodic nanowires (NW), whose power–law temperature dependence as a function of the NW cross-section area has a good agreement with the experimental results [211]. The direct conversion between thermal and electrical energies can be achieved by means of thermoelectric devices, whose performance can be measured using the dimensionless figure-of-merit defined as

$$ZT = \sigma S^2 T / (\kappa_{el} + \kappa_{ph}) \tag{9}$$

where *S* is the Seebeck coefficient; σ is the electrical conductivity; and κ_{el} and κ_{ph} are the electronic and phononic thermal conductivities, respectively [2]. The inherent correlation between these thermoelectric quantities makes difficult to improve the value of ZT. Recently, nanowire heterostructures, such as $M_2O_3/ZnO(M = In,G_a,F_e)$ with compositional segmentation, have demonstrated a significant improvement of ZT, mainly owing to the phonon scattering at composite interfaces [213]. Thermoelectricity in periodic and quasiperiodically segmented nanobelts and nanowires were comparatively studied within the Kubo-Greenwood formalism [214], and the results reveal the importance of segmentation in ZT as well as its further improvement when the quasiperiodicity is introduced, because it significantly diminishes the thermal conduction of long wavelength acoustic phonons, which are responsible for the thermal conductivity by phonons at low a temperature and do not feel local defects nor impurities [215]. Furthermore, branches of atoms attached to a nanowire may significantly modify the transport of excitations along it owing to wave interference, whose resonance produces zones of a very high value of ZT in the Hamiltonian parameter space [216]. Poly(C) DNA-like double chains, shown in Figure 2h, constitute another interesting example of branched low-dimensional systems, where the fishbone model and the two-site coarse grain model based on the Born potential including central and non-central interactions are used for the

calculation of electrical and lattice thermal conductivities, respectively, through the Kubo–Greenwood formula [217]. The results show the appearance of gaps in phononic transmittance spectra and a remarkable enhancement of ZT when periodic interfaces between poly(G) and poly(C) segments are introduced. Such ZT can be further improved by introducing a long-range quasiperiodic order, which avoids the thermal transport of numerous low-frequency phonons responsible of the lattice thermal conduction at a low temperature. Finally, the reservoirs have an important participation on the ZT, as they constitute the boundary conditions of the quantum system and may cause resonant interferences favoring the thermoelectric transport [210].

6. Conclusions

An aperiodic solid could be thermodynamically stable by the growth of entropy, the appearance of electronic energy gap around of the Fermi energy as occurred in the Peierls instability [218], or mechanisms described by the Hume–Rothery rules [219]. Such structural asymmetry represents a singular opportunity to achieve many unique physical properties. For example, the union of positively and negatively doped semiconductors constitutes the base of current microelectronics and modern illumination. Nevertheless, the presence of these structural interfaces requires new approaches for its study and design.

From the theoretical point of view, the tight-binding or Hubbard Hamiltonian based on the Wannier functions provides an atomic scale modelling of measurable physical quantities, where the huge degrees of freedom should be efficient and accurately addressed by taking the advantage of all visible and hidden symmetries. For instance, the exciton diffusion in organic solar cells has been recently analyzed by means of an attractive Hubbard Hamiltonian and the real-space renormalization method (RSRM) [220]. For aperiodic lattices with hierarchically structured inhomogeneities, the RSRM seems to be an ideal candidate because the structural scaling rule of these aperiodic lattices can be used as the starting point of RSRM. However, this procedure is truly useful only in 1D systems because they have a constant number of boundary atoms, in contrast to multidimensional systems whose boundary-atom number grows with the system size. These boundary atoms are extremely important for the Green's function determination, that is, a precise counting of all possible paths between two arbitrary atoms. For separable Hamiltonians, such as nearest-neighbor tight-binding Hamiltonian in cubically structured aperiodic lattices, a combination of the convolution theorem and RSRM has demonstrated its effectiveness [17]. Beyond cubically structured systems, the labyrinth lattice has been the first non-hypercubic aperiodic network recently addressed by the renormalization plus convolution scheme, where a new convolution theorem for a product of Hamiltonians instead of summation in the traditional convolution theorem was developed [184]. This fact opens a new horizon for the applicability of RSRM to more complex multidimensional aperiodic structures. On the other hand, the design of electronic and optical devices based on quantum mechanical calculations has been one of the biggest dreams of physicists and engineers, and the recent advances in RSRM bring it closer because these electronic and optical devices usually contain multiple aperiodic located structural interfaces. For example, first-principle calculations have been used in the multiscale design of omnidirectional dielectric reflectors [221] and Fabry-Perot resonators [222], whose results were experimentally confirmed.

Finally, despite the proven efficiency of RSRM in the study of systems with huge degrees of freedom, there are still many challenges in the development and application of new RSRM and they might be summarized as follows: (1) extend the applicability of RSRM to multidimensional lattices with complex structural symmetry; (2) combine the RSRM with the density functional theory to address multielectron systems; and (3) apply the RSRM to strong correlated phenomena, such as the superconductivity.

Author Contributions: V.S. and C.W. both participated in the conceptualization, reference analysis, figure preparation, manuscript writing, and final revision. All authors have read and agreed to the published version of the manuscript.

Funding: This research was partially supported by the Consejo Nacional de Ciencia y Tecnología of Mexico through grant 252943 and by the National Autonomous University of Mexico (UNAM) through projects PAPIIT-IN115519 and PAPIIT-IN110020. Computations were performed at Miztli of DGTIC, UNAM.

Acknowledgments: We would like to thank Antonio Galeote for his participation at early stages of this article and Fernando Sánchez for stimulating conversations and technical assistance.

Conflicts of Interest: The authors declare no conflict of interest.

Abbreviations

The following abbreviations are used in this manuscript:

YB	Yottabytes
RSRM	Real-space renormalization method
CPA	Coherent potential approximation
CPU	Central processing unit
1D	One-dimensional
2D	Two-dimensional
3D	Three-dimensional
DC	Direct current
AC	Alternating current
DOS	Density of states
IDOS	Integrated density of states
GF	Generalized Fibonacci
TM	Thue–Morse
PD	Period doubling
NW	Nanowires
IR	Infrared
DNA	Deoxyribonucleic acid
А	Adenine
С	Cytosine
G	Guanine
Т	Thymine

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