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# A transfer matrix method for the analysis of fractal quantum potentials

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## Abstract

The scattering properties of quantum particles on a sequence of potentials converging towards a fractal one are obtained by means of the transfer matrix method. The reflection coefficients for both the fractal potential and finite periodic potential are calculated and compared. It is shown that the reflection coefficient for the fractal potential has a self-similar structure associated with the fractal distribution of the potential whose degree of self-similarity has been quantified by means of the correlation function.

## 1. Introduction

Both quantum mechanics and elementary solid state physics courses illustrate the energy band structure in solids by means of the one-dimensional Kronig–Penney model that consists of a periodic configuration of square-well potentials [1, 2]. This problem is usually solved by matching the boundary conditions of the wavefunctions at the cell boundaries, thus requiring the computation of the determinant of a  $4 \times 4$  matrix [3]. Recently, some less tedious approaches have been proposed which usually can be readily adapted to finite periodic potentials [4]. Among these methods, those based on the transfer matrix approach [5], which only uses  $2 \times 2$  matrix operations in a purely algebraic way, are the most appropriate ones for beginners [6]. Moreover, this method allows us to introduce a numerical method based on a piecewise constant approximation for a general potential [7], the analysis of defects on otherwise periodic

potentials and even the consideration of more complicated potentials. Among the latter, fractal potentials are considered here.

In recent years the study of fractals has attracted much attention because many physical phenomena, natural structures and statistical processes can be analysed and described by using a fractal approach [8, 9]. From a mathematical point of view, fractals are self-similar structures obtained by performing a basic operation, called a generator, on a given geometrical object called an initiator, and repeating this process on multiple levels; in each one of them, an object composed of sub-units of itself is created that resembles the structure of the whole object. Mathematically, this property should hold on all scales. However, in the real world, there are necessarily lower and upper bounds over which such self-similar behaviour applies. Fractals are becoming a useful tool to model diverse physical systems [10, 11], and have new technological applications [12, 13].

In non-relativistic quantum mechanics, fractals have been used to generate new solutions of the Schrödinger equation which are continuous but nowhere differentiable wavefunctions [14], and models for the so-called fractal potentials [15]. Fractal potentials allow the analysis of quasi-periodic and nearly stochastic potentials using the symmetries induced by the self-similar structure of the potential. The simplest fractal, the (triadic) Cantor set, has been taken as a fractal potential for quantum scattering [16] and tunnelling [17, 18].

In this paper, we present a simple transfer matrix method to obtain the scattering properties of Cantor set fractal potentials, which can be easily automated by computers. The present method makes easier the comparison with the finite periodic case and shows how the reflection coefficient for the fractal case has a self-similar structure associated with the fractal distribution of the potential. The method can be easily implemented in any computer language, for example, the *Mathematica* software package, accessible to undergraduate students with only basic programming experience, so that it can be adopted for project assignments in computer physics courses. Starting with the implementation of the transfer matrix method for a potential barrier, the extension to finite periodic potentials is a straightforward one; its extension to Cantor set potentials can be based on a recursive implementation, involving the possible improvement of student programming skills. The inclusion of disorder in both the finite periodic and fractal potentials is straightforward and allows the interesting comparison of periodic, fractal and disordered systems, a topic suitable for advanced student assignments. Furthermore, these projects can introduce the student to the analysis of computational complexity of algorithms, since the Cantor set pre-fractal has a large number of potential barriers and its simulation requires an exponential number of matrix products if not programmed properly.

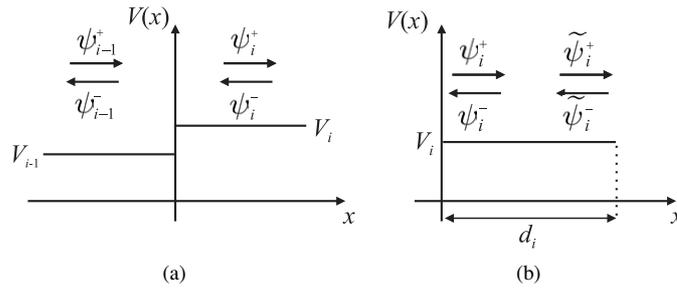
The contents of this paper are as follows. The following section recalls the main facts about the transfer matrix method for quantum scattering implemented by piecewise constant potentials. In section 3, the reflection coefficient for the tunnelling on both finite periodic and Cantor set pre-fractals is determined and compared. Finally, the last section is devoted to the main conclusions.

## 2. Presentation of the problem

Let us consider the one-dimensional, steady-state, linear Schrödinger equation

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x)\psi(x) = E\psi(x), \quad (1)$$

where  $\psi(x)$ ,  $m$  and  $E$  are the particle wavefunction, mass and energy, respectively,  $\hbar$  is Planck's constant and  $V(x)$  is the quasi-periodic potential which can be represented by a piecewise constant function. Figure 1(a) shows the quantum scattering at the  $i$ th interface



**Figure 1.** (a) Local scattering with the  $i$ th interface of the piecewise constant potential among the values  $V_{i-1}$  and  $V_i$ . (b) Wavefunction propagation through the constant potential  $V_i$  used to calculate the propagation matrix.

between two successive constant values of the piecewise potential, whose position, without loss of generality, has been taken as  $x = 0$ . In this figure, both  $\psi_i^+$  and  $\psi_i^-$  are forward and backward, respectively, plane wavefunctions on the region where the potential value is  $V_i$ , so  $\psi_i = \psi_i^+ + \psi_i^-$  there and

$$\psi_i^\pm = A_i^\pm e^{\pm ik_i x}, \quad k_i = \frac{1}{\hbar} \sqrt{2m(E - V_i)}, \quad (2)$$

where  $i = \sqrt{-1}$ ,  $k_i$  is the local particle momentum and  $A_i^\pm$  are integration constants to be determined by applying the standard boundary conditions at the interface, the continuity of both the wavefunction and its derivative, i.e.,

$$\begin{aligned} \psi_{i-1}(x=0) &= \psi_i(x=0), & A_{i-1}^+ + A_{i-1}^- &= A_i^+ + A_i^-, \\ \psi'_{i-1}(x=0) &= \psi'_i(x=0), & k_{i-1}A_{i-1}^+ - k_{i-1}A_{i-1}^- &= k_iA_i^+ - k_iA_i^-, \end{aligned} \quad (3)$$

where the prime denotes differentiation. Equation (3) is a linear system of equations easily written in matrix notation as

$$\begin{pmatrix} 1 & 1 \\ k_{i-1} & -k_{i-1} \end{pmatrix} \begin{pmatrix} A_{i-1}^+ \\ A_{i-1}^- \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ k_i & -k_i \end{pmatrix} \begin{pmatrix} A_i^+ \\ A_i^- \end{pmatrix}, \quad (4)$$

and yielding

$$\begin{pmatrix} A_{i-1}^+ \\ A_{i-1}^- \end{pmatrix} = D_{i-1}^{-1} D_i \begin{pmatrix} A_i^+ \\ A_i^- \end{pmatrix}, \quad D_i = \begin{pmatrix} 1 & 1 \\ k_i & -k_i \end{pmatrix}. \quad (5)$$

Hereon, the matrix  $D_{i-1}^{-1} D_i$  is referred to as the wave scattering matrix.

After crossing the  $i$ th interface, the plane wavefunction propagates through the constant potential  $V_i$  until finding the next interface at a distance  $d_i$ . Using the notation shown in figure 1(b), this wavefunction is

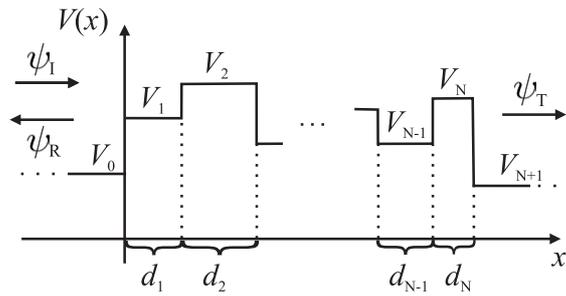
$$\tilde{\psi}_i^\pm = A_i^\pm e^{\pm ik_i d_i} e^{\pm ik_i x} = \tilde{A}_i^\pm e^{\pm ik_i x}, \quad (6)$$

and a wave propagation matrix  $P_i$  can be defined as

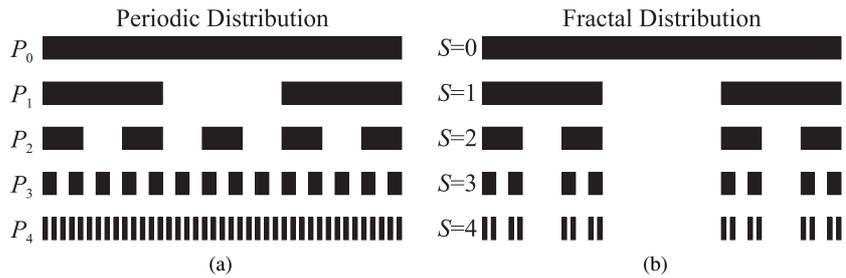
$$\begin{pmatrix} \tilde{A}_{i-1}^+ \\ \tilde{A}_{i-1}^- \end{pmatrix} = \begin{pmatrix} e^{ik_i d_i} & 0 \\ 0 & e^{-ik_i d_i} \end{pmatrix} \begin{pmatrix} A_i^+ \\ A_i^- \end{pmatrix} = P_i \begin{pmatrix} A_i^+ \\ A_i^- \end{pmatrix}. \quad (7)$$

Both the scattering and propagation matrices can be used to solve the general problem of the scattering with a piecewise constant potential with  $N$  potential wells, as shown in figure 2. The successive application of the scattering and propagation matrices yields

$$\begin{pmatrix} A_0^+ \\ A_0^- \end{pmatrix} = D_0^{-1} D_1 \begin{pmatrix} A_1^+ \\ A_1^- \end{pmatrix} = D_0^{-1} D_1 P_1 D_1^{-1} D_2 \begin{pmatrix} A_2^+ \\ A_2^- \end{pmatrix}, \quad (8)$$



**Figure 2.** Piecewise constant potential with  $N$  potential wells  $V_i$  with  $d_i$  as the corresponding width.  $V_0$  and  $V_{N+1}$  are the surrounding constant potential values extended to infinity.



**Figure 3.** Finite periodic (a) and Cantor set quasi-periodic (b) potentials where the white and black regions denote the potential values 0 and  $\mathcal{V}$ , respectively.

and, in the most general form,

$$\begin{pmatrix} A_0^+ \\ A_0^- \end{pmatrix} = M \begin{pmatrix} A_{N+1}^+ \\ A_{N+1}^- \end{pmatrix}, \quad M = D_0^{-1} \left( \prod_{i=1}^N D_i P_i D_i^{-1} \right) D_{N+1}. \tag{9}$$

Both the reflection and transmission coefficients of the scattering of a quantum particle, incoming from the left, with the  $N$ -well potential are determined by the coefficients of the matrix  $M$ ,

$$\begin{pmatrix} A_0^+ \\ A_0^- \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} A_{N+1}^+ \\ 0 \end{pmatrix}, \tag{10}$$

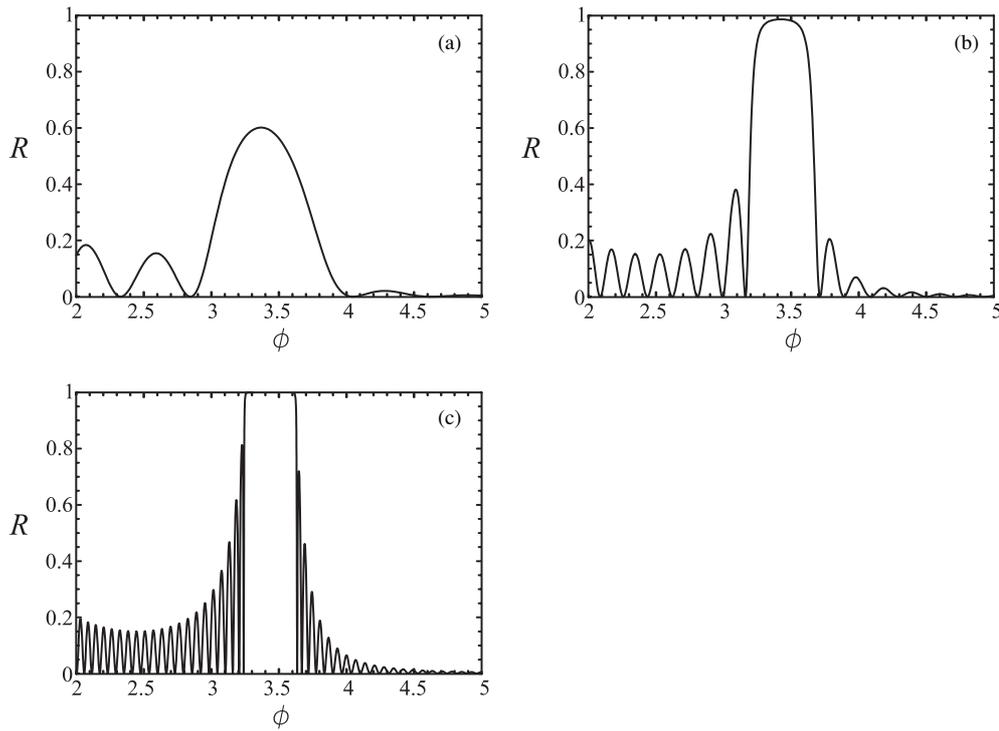
where no backward particle can be found on the right side of the potential, so  $A_{N+1}^- = 0$ . Both the reflection and transmission coefficients [2] are given by

$$R = \frac{|A_0^-|^2}{|A_0^+|^2} = \frac{|M_{21}|^2}{|M_{11}|^2}, \quad T = \frac{k_{N+1} |A_{N+1}^+|^2}{k_0 |A_0^+|^2} = \frac{k_{N+1}}{k_0 |M_{11}|^2}, \tag{11}$$

respectively.

### 3. Presentation of results

The simplest fractal potential is the (triadic) Cantor set, shown in figure 3(b), which can be obtained by means of an iterative construction. The first step ( $S = 0$ ) is to take a segment of unit length. The next one ( $S = 1$ ) is to divide the segment into three equal parts of length  $1/3$  and remove the central one. In general, at the stage  $S$ , there are  $2^S$  segments of length  $3^{-S}$



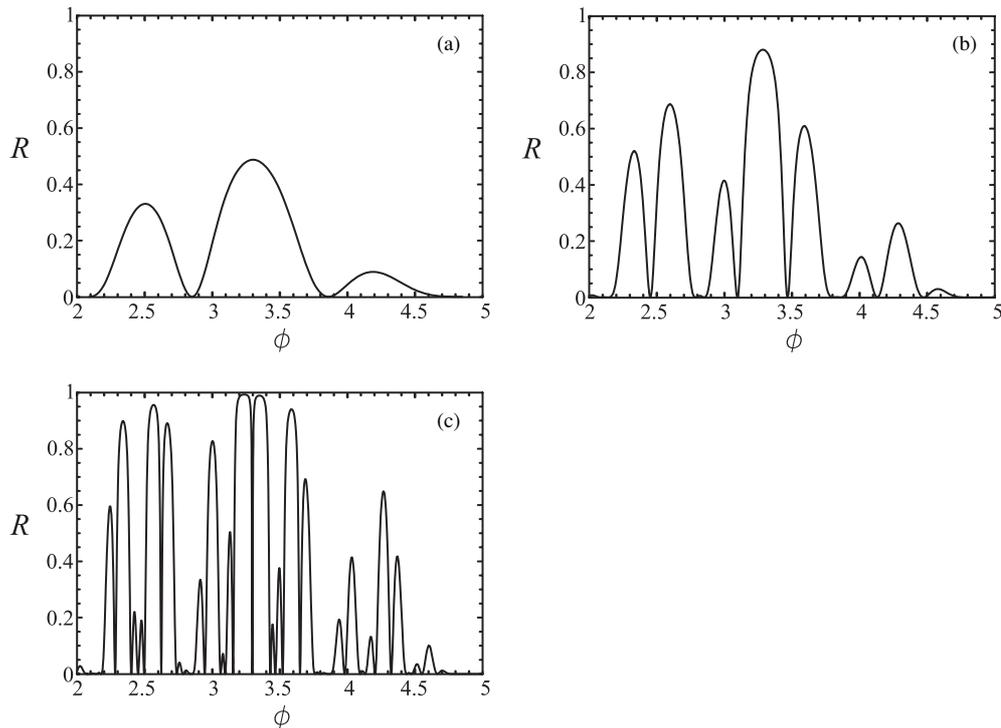
**Figure 4.** Scattering reflection coefficient for the finite periodic potentials of stages  $p_2$  (a),  $p_3$  (b) and  $p_4$  (c) as a function of the normalized energy  $\phi$  for the potential  $\phi_V = 2$ .

with  $2^S - 1$  gaps in between. Stage  $S + 1$  is obtained by dividing each of these segments into three parts of length  $3^{-S-1}$  and removing the central ones. In figure 3(b), only the four first stages are shown for clarity. Note that the  $S$ th stage Cantor set pre-fractal can be interpreted as a quasi-periodic distribution of segments which can be obtained by removing some segments in a finite periodic distribution as shown in figure 3(a). This distribution at stage  $p_M$  has  $(3^M - 1)/2 + 1$  potential barriers of length  $3^{-M}$ , separated by potential wells of the same length, so the ‘period’ of this finite structure is  $\Lambda = 2 \times 3^{-M}$ .

The scattering problem for both the quasi-periodic, Cantor set, pre-fractal potential, and the finite periodic potential can be easily solved by means of the matrix transfer theory presented earlier in this paper. It is standard to normalize both the energy and the height of the potential barrier by the period  $\Lambda$ , introducing the non-dimensional variables

$$\phi = \Lambda \frac{\sqrt{2mE}}{\hbar}, \quad \phi_V = \Lambda \frac{\sqrt{2mV}}{\hbar}.$$

Figures 4 and 5 show the reflection coefficient,  $R$ , for the finite periodic potential and Cantor set fractal potential, respectively, around the interval which contains the first bandgap of the infinite periodic one. Using the standard Kronig–Penney model [19], this bandgap can be numerically calculated, being located between the values  $3.2519 < \phi < 3.6222$  for the potential  $\phi_V = 2$ . In this energy range, a Bloch wavefunction does not propagate in an infinite periodic potential and, therefore, the transmission coefficient ideally vanishes ( $R = 1$ ); only evanescent wavefunctions characterized by a complex wavevector,  $k$ , are solutions of the Schrödinger equation. For this reason, when the number of periods is finite, the quantum

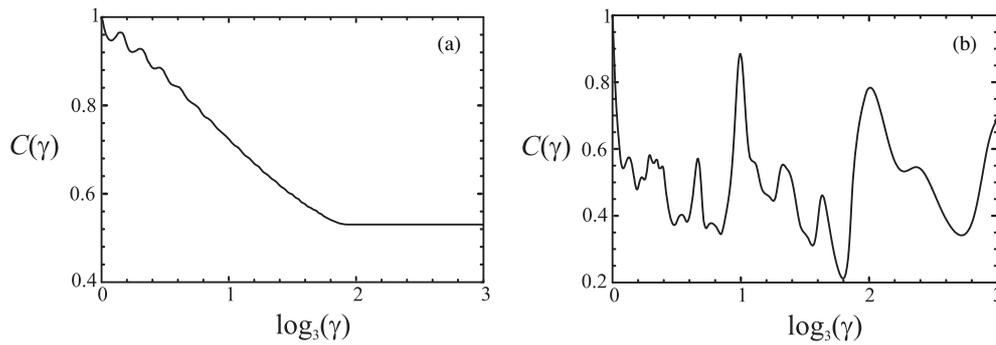


**Figure 5.** Scattering reflection coefficient for the Cantor set pre-fractal potentials of stages  $S = 2$  (a),  $S = 3$  (b) and  $S = 4$  (c) as a function of the normalized energy  $\phi$  for the potential  $\phi_\gamma = 2$ .

particle may pass through the potential distribution by the tunnelling effect. Figure 4 shows that the reflection coefficient approaches unity as the number of periods in the spatial interval increases, thus illustrating the process of appearance of the bandgap of the (full) periodic structure. The value  $R = 1$  is never reached in the finite periodic structure, but, even for  $p_4$ , the graphical resolution of figure 4 is unable to highlight this fact.

Figure 5 shows the reflection coefficient for the Cantor set pre-fractal potential for  $S = 2$  (a),  $S = 3$  (b) and  $S = 4$  (c). It is shown that the reflection at each higher stage is a modulated version of that associated with the previous stage. That is, the reflection spectrum exhibits a characteristic fractal profile that reproduces the self-similarity of the potential distribution. In fact, any wide peak at stage  $S$  is transformed into three narrower and taller peaks at stage  $S+1$ . Zero reflection from these fractal quantum potential occurs at specified discrete energies, while near total reflection is possible at other discrete energies. Comparing figures 4 and 5, an increasing number of zeros inside the bandgap is observed. These zeros represent resonances due to the presence of ‘defects’ in the quasiperiodic potential obtained by removing some segments in the finite periodic sequence. In the limit  $S \rightarrow \infty$ , the reflection coefficient for Cantor set pre-fractals approaches unity with very narrow resonances in the interval shown in figure 5.

In order to quantify the self-similarity of the reflection coefficient for the fractal potential shown in figure 5, the correlation coefficient defined by Sakurada *et al* [20] is used. A general function  $f(x)$  is self-similar with respect to a point  $x_0$  in its domain, cf  $[x_1, x_2]$ , if it remains unchanged when rescaling its domain with  $x_0$  fixed, i.e., if  $f(x_0 + (x - x_0)/\gamma) = \gamma^\alpha f(x)$ , where  $\gamma$  is a scaling factor and  $\alpha$  is the scaling exponent. Thus, the correlation coefficient



**Figure 6.** Correlation function  $C(\gamma)$  for the reflection coefficients shown in figures 4(c) (a) and 5(c) (b).

with respect to the point  $x_0$  is defined by

$$C(\gamma) = \frac{\int_{x_1}^{x_2} f(x) f(x_0 + (x - x_0)/\gamma) dx}{\sqrt{\int_{x_1}^{x_2} f^2(x) dx \cdot \int_{x_1}^{x_2} f^2(x_0 + (x - x_0)/\gamma) dx}}$$

Note that  $C(\gamma) = 1$  for a self-similar function with respect to  $x_0$ .

Figure 6 shows the correlation coefficient of the reflection coefficient for both the periodic and fractal potential of stages  $p_4$  and  $S = 4$ , respectively, using as integration interval the domain used in figures 4(c) and 5(c). Note that a logarithmic scale in base 3 has been used for the horizontal axis. The local maxima of the correlation function for the fractal potential, cf figure 6(b), located at  $\gamma = 3$  and 9, clearly show the self-similarity of the reflection coefficient as a consequence of the fractal structure of the potential. For comparison, the correlation function for the periodic potential, cf figure 6(a), does not show significant local maxima, except for the small modulation for small  $\gamma$  due to the lateral lobes around the bandgap, confirming that the reflection coefficient is not self-similar in this case. The constant value of the correlation function for  $\gamma > 8$  is an artefact due to the integration window, since, for these scalings, the constant value on the bandgap fills the interval completely.

#### 4. Conclusions

The transfer matrix method is becoming the standard method for the calculation of the tunnelling of quantum particles on constant piecewise potentials because it can be used for simple textbook-like problems and as a numerical method for computer simulations. This procedure has been applied to Cantor set fractal potentials, which are constant value potentials with support on a Cantor set. For pre-fractals, cf the  $S$ th stage fractal, the reflection coefficient was numerically calculated and compared with that of a finite periodic potential of the same period. The appearance of the first bandgap of the Kronig–Penney model in the finite periodic potential has been illustrated. The reflection coefficient for the Cantor set potential is self-similar as shown quantitatively by means of the correlation function.

The transfer matrix method presented in this paper can be easily adopted in computer laboratories for undergraduate quantum mechanics courses, providing a powerful method for developing students' skills on physics by means of computational tools. Furthermore, fractal geometry is a highly motivating topic for students providing a great opportunity for the students to undertake projects closely related to research ones.

For advanced seminars, the incorporation of disorder in both the finite periodic and fractal potentials by stochastically perturbing the distance between the barriers and their width must be considered. Theoretical results for disordered Kronig–Penney models, as those presented in chapter 8 of Ziman’s monograph [6] for the density of states, can also be incorporated in these projects.

Finally, note that the transfer matrix method can also be extended to both other one-dimensional fractals, such as polyadic Cantor sets, and, with the proper extensions, to other two-dimensional ones.

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