Transport and optical properties of an electron gas in a Sierpinski carpet

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Recent progress in the design and fabrication of artificial two-dimensional (2D) materials paves the way for the experimental realization of electron systems moving on plane fractals. In this work, we present the results of computer simulations for the conductance and optical absorption spectrum of a 2D electron gas roaming on a Sierpinski carpet, i.e. a plane fractal with Hausdorff dimension intermediate between one and two. We find that the conductance is sensitive to the spatial location of the leads and that it displays fractal fluctuations whose dimension is compatible with the Hausdorff dimension of the sample. Very interestingly, electrons in this fractal display a broadband optical absorption spectrum, which possesses sharp “molecular” peaks at low photon energies.

Introduction.— A variety of experimental protocols that can be used to create artificial two-dimensional (2D) lattices for electrons, atoms, and photons are nowadays available. Examples include schemes for creating artificial honeycomb lattices [1], where a wealth of interesting phenomena have been observed such as Mott-Hubbard split bands [2], massless Dirac fermion behavior modified by pseudo-electric and pseudo-magnetic fields [3], and photonic Floquet topological insulating states [4]. In the case of ultracold atomic gases loaded in honeycomb optical lattices, recent progress has even led to the experimental realization [5] of the Haldane model [6].

In the solid state, a combination of e-beam nanolithography, etching, and metallic gate deposition [7–11] can in principle yield high quality two-dimensional (2D) patterns with arbitrary shape in semiconductor heterostructures (such as GaAs/AlGaAs) hosting ultra-high mobility 2D electron gases (EGs). Ultimately, these procedures yield an external potential landscape with the desired geometry that acts as a lattice of potential wells to trap electrons. The spatial resolution of these techniques can reach values of a few tens of nanometer or even below. Further improvements in spatial resolution can be obtained by bottom-up nanofabrication methods such as nanocrystal self-assembly [12]. These approaches allow to independently control the electron density and intersite distances and to tune the interplay between on-site and nearest-neighbor repulsive interactions and single-particle hopping, opening the way to the observation of collective phenomena and quantum phase transitions in such artificial solid-state systems [2]. Synthetic solid-state quantum materials can also be created by utilizing scanning probe methods [3]. Here, suitably chosen molecules can be positioned with atomic precision on top of a substrate (such as Cu) with the aid of the tip of a scanning tunneling microscope (STM). Electrons confined in the substrate surface states and subject to the potential created by the deposited molecules can be probed via STM measurements [3].

These experimental achievements motivate the theo-
retical investigation of complex 2D structures, with the aim of discovering novel transport and optical features which could enable or improve technological applications. In this work we present a theoretical study of the transport and optical properties of a 2DEG in a Sierpinski carpet (SC), which is a self-similar 2D structure [13] shown in Fig. 1. The self-similarity of the SC is mathematically quantified by the fact that its Hausdorff dimension [13] \(d_H\) (i.e. a generalization of the topological dimension) is between one (a line) and two (a plane), which makes the SC a fractal [14].

While brownian motion and the heat diffusion equation on fractal geometries have been extensively studied in the literature [15, 16], the transport and optical properties of electrons roaming on such complicated geometrical structures have comparatively received less attention. More precisely, some analytical [17, 18] and numerical [19–22] studies of the conductance of electrons in Sierpinski fractals have appeared in the literature. We are instead unaware of studies of the optical properties of electron systems in fractals, with the exception of an experimental work [23] on a one-dimensional potential in (Al,Ga)As heterostructures.

In this work we show that extended states, which lead positions and their widths, and it displays fractal number of open channels in the leads, depending on the potential and optical properties of a magnetic field. We show that extended states, which are responsible for large conductance values, are quite different from that of a quantum particle displaying a self-similar spectrum. Such problems are very well studied in physics, a paradigmatic example being that of the Hofstadter butterfly spectrum [26] displayed by an electron moving in 2D under the combined effect of a periodic potential and a perpendicular magnetic field. Finally, we are not interested in the distribution of eigenvalues and nature of the corresponding eigenstates of electrons in plane fractals, which have been studied in great detail [27–31]. Rather, our aim is to unveil fundamental dc and ac transport characteristics, which can be measured with current technology.

Model and methods.—We describe a 2DEG in a SC by means of a single-orbital tight-binding Hamiltonian of the form

\[
\mathcal{H} = -t \sum_{\langle i,j \rangle,\sigma} (c_{i,\sigma}^\dagger c_{j,\sigma} + \text{H.c.}).
\]

This describes electrons with spin \(\sigma = \uparrow, \downarrow\) hopping between the nearest-neighbor sites \(\langle i,j \rangle\) of a SC with Hausdorff dimension \(d_H = \log_2 N,\) as explained in Fig. 1. With reference to Fig. 1, each discretized SC sample is characterized by two integers, \(\{n, m\}.\) In this work \(n = 2,\) while \(m\) varies from \(m = 2\) to \(m = 8.\) The Hamiltonian (1) is particle-hole symmetric and the spectrum of eigenvalues extends from \(-4t\) to \(4t\) for a bandwidth equal to \(8t.\)

The hopping parameter \(t\) is used below as unit of energy. Nanopattering a SC on the surface of semiconductor hosting a high mobility 2DEG is expected [2, 7, 8] to yield \(t\) of the order of a few meV, while protocols based on STM manipulation [3] are expected to yield \(t \sim 100\) meV. For the sake of simplicity, we ignore magnetic fields and electron-electron interactions, which are expected to lead to very interesting quantitative and qualitative effects that will be the subject of future works.

The conductance and wavefunction calculations are performed by using kwant [32]. In this toolkit, wavefunction matching is implemented to compute the wavefunctions in the scattering region and the scattering matrix \(S_{nm}\) for an incoming propagating mode \(n\) and an outgoing mode \(m.\) The conductance between the left lead \(L\) and the right lead \(R\) is given by the Landauer formula

\[
G = \frac{2e^2}{h} \sum_{n \in L, m \in R} |S_{nm}|^2. \tag{2}
\]

The density of states (DOS) \(\nu(E)\) and optical conductivity \(\sigma(\omega)\) are calculated by using the tight-binding propagation method (TBPM) [33, 34]. Since TBPM does not involve diagonalization of matrices, both CPU time and memory cost grown linearly with the sample size, allowing calculations with up to \(10^{10}\) sites.

In TBPM, the DOS is obtained by the following Fourier transform [33–35]

\[
\nu(E) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp(iE\tau/h) \langle \varphi|\varphi(\tau)\rangle d\tau, \tag{3}
\]

where the initial state \(\varphi = \sum_i a_i|i\rangle\) is a superposition of localized orbitals \(|i\rangle\) with complex random coefficients \(a_i\) and the wave propagation \(\varphi(\tau) = \exp(-i\mathcal{H}\tau/h)|\varphi\rangle\) is performed numerically by using the Chebyshev polynomial algorithm. Our results for the DOS of a \{2,3\} SC are reported in Fig. 1b). We have checked that the function \(\nu(E)\) rapidly converges for a fixed value of \(n\) and increasing \(m:\) for example, results for the \{2,7\} and \{2,8\} SCs (not shown) are nearly indistinguishable over the entire bandwidth.

Quantum transport and fractal conductance fluctuations.—We have calculated the energy dependence of the two-terminal conductance \(G(E)\) of the tight-binding model (1), for two different lead configurations, as in Figs. 1c) and d).
A summary of our main results for a \{2,3\} SC is reported in Fig. 2. In panel a) we clearly see that the two-terminal conductance $G(E)$ is equal to $4e^2/h$ for $E = 0$, where a conductive extended state is present [17]. This is because for the two leads positioned as in Fig. 1c), electrons of a given spin injected on the left side of the sample can reach the right side by following two equivalent paths, Fig. 2c), each carrying a conductance quantum, without being backscattered by the inner holes of the SC. On the other hand, as we can see from panel b), the sample can be insulating (i.e. $G = 0$), at the same energy when probed with the leads positioned as in Fig. 1d).

Data in Fig. 2 display also wild fluctuations. Such conductance fluctuations (CFs) can be quantified by using a box-counting (BC) algorithm [36]. This counts the number $N$ of squares of size $\delta$, which is necessary to continuously cover the graph of $G(E)$ (in units of $e^2/h$) rescaled to a unit square. In general, points in the plane $(\log N, -\log \delta)$ are expected to fall in three distinct regions. For large values of $\delta$, the squares are too large to distinguish the features of the graph and $N$ grows slowly as $\delta$ decreases. For very small values of $\delta$, the squares are so small that they resolve the single points in the set of data belonging to the CF graph: in this case $N$ is expected to saturate to the number $N_s$ of points in the energy mesh where $G(E)$ is evaluated. Finally, there is an intermediate region (usually called “scaling region”) where scaling is linear in the log-log plane, i.e. where $N \sim \delta^{-d}$. The slope $d$ in the scaling region is the BC estimate of the Hausdorff dimension of the CFs.

In Fig. 3, we show the results of the BC algorithm for the CFs of two SC samples with (slightly) different Hausdorff dimensions, obtained by changing $N$ and $L$ in the iterative geometrical construction illustrated in Fig. 1a). Results do not depend on the spatial arrangement of the leads. The analyzed CFs clearly show fractal behavior over a scaling region of more than two orders of magnitude. Fractal CFs emerge [24] in the problem of phase-coherent ballistic transport and in the presence to strong quantum localization [36]. Indeed, in the SC transport problem, almost all wavefunctions are localized [28] [see e.g. Fig. 2d)] and do not contribute to transport (even in the absence of elastic disorder) due to scattering of electrons against the inner holes.

Finally, we note that the value of $d$ extracted from our numerical analysis is in excellent agreement with the Hausdorff dimension $d_H$ of the corresponding SC sample [37]. It is remarkable that the analysis of CFs carries information on the sample geometry, down to very small length scales.

Fig. 4 shows that the conductance of the 2DEG in a SC is robust with respect to both localized [panel a)] and smooth [panel b)] elastic disorder. The impact of a single-site vacancy—located on the highly-conductive path through the bulk of the SC displayed in Fig. 2c)—is shown in Fig. 4a). We see that, despite such a strong, localized disorder source, $G(E)$ still reaches its maximum value $G(E) = 4e^2/h$ at $E = 0$. The impact of a smooth disorder potential,

$$ V = \sum_i \delta \mu(r_i)c_i^\dagger c_i \ ,$$  \hspace{1cm} (4)

which varies on an energy scale equal to 20% of the hopping amplitude, is shown in Fig. 4b). The spatial variations of $\delta \mu(r_i)/t$ are reported in Fig. 4c), while the fate of the highly-conductive bulk path shown in Fig. 2c) is
illustrated in Fig. 4d).

Optical conductivity.—We have calculated the optical conductivity from the Kubo formula for the current response function to a uniform time-dependent vector potential. In the TBPM, this is calculated (omitting the Drude contribution at \( \omega = 0 \)) from [33, 34]:

\[
\text{Re}[\sigma(\omega)] = \frac{1}{S} \lim_{\epsilon \to 0^+} \frac{e^{-\beta \hbar \omega} - \frac{1}{\omega} \int_0^\infty e^{i \epsilon \tau} \sin (\hbar \omega \tau)}{\omega} \times 2 \text{Im} \langle \varphi | f(\mathcal{H}) J(\tau) [1 - f(\mathcal{H})] J(\varphi) \rangle d\tau ,
\]

where \( S \) is the sample area, \( \beta = 1/(k_B T) \) is the inverse temperature, \( f(\mathcal{H}) = 1/[e^{\beta(\mathcal{H} - \mu)} + 1] \) is the Fermi-Dirac distribution operator, and \( J(\tau) = e^{i \mathcal{H} \tau / \hbar} e^{-i \mathcal{H} \tau / \hbar} \) is the current operator in the Heisenberg picture of the time evolution.

Fig. 5a shows that the dependence of the absorption spectrum Re[\( \sigma(\omega) \)] (in units of \( e^2/h \)) on the photon energy \( \hbar \omega \) (in units of \( t \)). This quantity is evaluated at a finite but small temperature \( k_B T \ll t \) (specifically, \( k_B T = 0.0034t \)) and for two SC samples, i.e. \{2, 3\} and \{2, 8\}. By looking at the difference between Re[\( \sigma(\omega) \)] at \( m = 7 \) (not shown) and \( m = 8 \) (and fixed temperature), we conclude that the data shown for \( m = 8 \) represent the \( m \to \infty \) result. We note that the optical absorption spectrum features three distinct behaviors. For photon energies \( \hbar \omega \ll 0.2t \), absorption is very large, with Re[\( \sigma(\omega) \)] \( \gg e^2/h \), peaking at \( \approx 25e^2/h \). The peak value is quite sensitive to the value of \( n \) in a \( \{n, m\} \) SC: for example, this peak reaches \( \approx 40e^2/h \) in a \( \{4, 8\} \) SC. For photon energies \( 0.2t \ll \hbar \omega \ll 0.5t \), Re[\( \sigma(\omega) \)] features a plateau at a value which is intermediate between \( 5e^2/h \) and \( 10e^2/h \). Finally, an exponential tail Re[\( \sigma(\omega) \)] \( \propto e^{-\alpha(\hbar \omega / t)} \) with \( \alpha \approx 1.5 \) kicks in for \( \hbar \omega > 0.5t \).

For a choice of the hopping amplitude \( t = 100 \text{ meV} \) (which is the expected value for a SC realized by STM manipulation [3]), the absorption of the SC vanishes in the visible range of the electromagnetic spectrum and it is of the order of \( e^2/h \) in the infrared. For photon frequencies spanning the range \( 300 \text{ GHz} \leq f \leq 5 \text{ THz} \) the real part of the optical conductivity is very large, much
larger than $e^2/h$, and displays a sequence of molecular resonances (whose smoothness is controlled by temperature).

**Summary.**—In this work we have carried out extensive computer simulations of the conductance and optical absorption spectrum of a two-dimensional electron gas roaming on a prototypical plane fractal, the Sierpinski carpet. We have demonstrated that the conductance is sensitive to the spatial location of the leads and that it displays fractal fluctuations whose dimension is compatible with the Hausdorff dimension of the sample. Due to the presence of a massive number of localized eigenstates, the optical absorption spectrum turns out to display sharp molecular peaks at low photon energies, which may pave the way for applications in sensing and plasmonics.

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[24] R. Ketzmeric, *Phys. Rev. B* **54**, 10841 (1996).

[25] R. Taylor, R. Newbury, A. Micolich, M. Fromhold, H. Linke, G. Davies, J. Bird, T. Martin, and C. Marlow, *A review of fractal conductance fluctuations in ballistic semiconductor devices*, in *Electron transport in quantum dots*, edited by J.P. Bird (Kluwer Academic Publishers, 2003).

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

[27] R. Rammal and G. Toulouse, *Phys. Rev. Lett.* **49**, 1194 (1982).

[28] E. Domany, S. Alexander, D. Bensimon, and L.P. Kadanoff, *Phys. Rev. B* **28**, 3110 (1983).

[29] R. Rammal, *Phys. Rev. B* **28**, 4871(R) (1983).

[30] X.R. Wang, *Phys. Rev. B* **51**, 9310 (1995).

[31] A. Hernando, M. Šulc, and J. Vanček, *arXiv*:1503.07741.

[32] C.W. Groth, M. Wimmer, A.R. Akhmerov, and X. Waintal, *New J. Phys.* **16**, 063065 (2014).

[33] S. Yuan, H. De Raedt, and M.I. Katsnelson, *Phys. Rev. B* **82**, 115448 (2010).

[34] S. Yuan, R. Roldán, H. De Raedt, and M.I. Katsnelson, *Phys. Rev. B* **84**, 195418 (2011).

[35] A. Hams and H. De Raedt, *Phys. Rev. E* **62**, 4365 (2000).

[36] I. Guarneri and M. Terraneo, *Phys. Rev. E* **65**, 015203(R) (2001).

[37] The Hausdorff dimensions of the SCs used to produce the results in Figs. 3a) and b) differ by only 5%. To further corroborate the conjecture \( d = d_H \) one needs to carry out a more detailed data analysis in which SCs with larger values of \( \mathcal{N} \) are used. This lowers the fractal dimension and can help finding deviations from the conjecture \( d = d_H \). Such a detailed numerical investigation requires the simulation of large samples, which is quite demanding, and lies outside the scope of the present work.