

A FRACTAL QUANTUM MECHANICAL MODEL WITH COULOMB POTENTIAL

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ABSTRACT. We study the Schrödinger operator $H = -\Delta + V$ on the product of two copies of an infinite blowup of the Sierpinski gasket, where V is the analog of a Coulomb potential (ΔV is a multiple of a delta function). So H is the analog of the standard Hydrogen atom model in nonrelativistic quantum mechanics. Like the classical model, we show that the essential spectrum of H is the same as for $-\Delta$, and there is a countable discrete spectrum of negative eigenvalues.

1. Introduction. Nonrelativistic quantum mechanics may be viewed as the study of the Schrödinger operator

$$H = -\Delta + V \tag{1.1}$$

on Euclidean space. On any space where a Laplacian may be defined, it makes sense mathematically to consider the analog of (1.1), whether or not there is any physical interpretation of the resulting theory. Indeed there are many such spaces, including the fractals studied here, where there is no obvious analog of classical mechanics.

We will work with fractals built from the Sierpinski gasket (SG) and the Laplacian on SG constructed by Kigami (see [17] and [25] for accounts of this construction). Since SG is the analog of the unit interval, we will first need to blowup SG to K_∞ , the analog of the line, and then take products to obtain the analog of Euclidean space. The theory of Laplacians in these contexts is developed in [26] and [24]. Other work on quantum mechanical analogs in the fractal context includes [20] and [19] on the Heisenberg uncertainty principle, [21] on eigenvalue clusters, [12] on square-well potentials, and [14] on harmonic oscillators.

In this paper we study the analog of the Coulomb potential in 3-space which gives the Hydrogen atom model that is discussed in every book on quantum mechanics. This model can be solved explicitly, while the fractal analogs cannot (perhaps it is better to say that it seems implausible that explicit solutions will be discovered in the near future). Thus we will be more interested in the general theoretic development of Schrödinger operators as presented in the books of Reed and Simon [22] (see also [13]), as these developments allow one to obtain the following conclusions without having to know the explicit solutions:

- (i) the operator is self-adjoint and bounded below;

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- (ii) the essential spectrum is the same as for the free Hamiltonian $-\Delta$ (in this case $[0, \infty)$);
- (iii) there are a countable number of discrete eigenfunctions with eigenvalue below the bottom of the essential spectrum (negative eigenvalues).

Our goal is to obtain analogous results in the fractal setting, as well as to estimate the counting function for the negative eigenvalues in (iii) above. We note also that the spectrum of $-\Delta$ in (ii) consists of discrete eigenvalues with infinite multiplicity, or more precisely the closure of this set of eigenvalues. Presumably these eigenspaces split into eigenvalue clusters, so that there will be nonessential positive eigenvalues. Our methods do not rule out the occurrence of singular continuous spectrum for H .

To begin our investigation we need to address the question: what potentials V should we choose to be the analogs of the Coulomb potentials $-c|x - \bar{x}|^{-1}$ in \mathbb{R}^3 for \bar{x} a point in \mathbb{R}^3 and c a positive constant? (Note that we choose a negative coefficient in order to have an attracting force as in the Hydrogen atom.) While there may be other ways of looking at this question, we observe simply that the Coulomb potentials have two basic properties:

- (a) ΔV is a multiple of a delta function;
- (b) V vanishes at infinity.

Moreover, these properties characterize the Coulomb potentials. Indeed, if $\Delta V = \Delta V'$ and both V and V' vanish at infinity, then $V - V'$ is harmonic and vanishes at infinity, hence must be identically zero.

With this in mind, we propose to define a Coulomb potential on any noncompact space with a Laplacian to be a function V satisfying (a) and (b) above. Note that (a) allows two parameters, one being the point where the delta function is concentrated, and one being the constant multiple. Since harmonic functions will satisfy a maximal principle in any reasonable theory, condition (b) will uniquely determine the potential once these parameters are chosen. Of course, not every space will have Coulomb potentials: for Euclidean space \mathbb{R}^N with standard Laplacian, there are no Coulomb potentials for $N = 1$ or 2 . Also, for $N \geq 4$, the Hamiltonian H with Coulomb potential will not satisfy conditions (i), (ii), (iii) above. Thus, with our definition, only dimension $N = 3$ has a satisfactory theory. This might lead some readers to prefer a different definition; perhaps $V(x) = -c d(x, \bar{x})^{-1}$ for some canonical metric d on the space. The trouble with this approach is that on many interesting spaces we might not have any canonical metric, even though we might be able to come up with a Lipschitz equivalence class of metrics that is in some sense natural. In the fractal setting, we could argue that the effective resistance metric on K_∞ is canonical, but this does not help when we pass to products.

The advantage of defining Coulomb potentials by (a) and (b) is that the nature of fundamental solutions of the Laplacians as called for in (a) is one of the first questions that will be addressed in any theory. In particular, if one has a heat kernel $h_t(x, y)$ (representing $e^{t\Delta}$), then

$$V(x) = -c \int_0^\infty h_t(x, y) dt \quad (1.2)$$

will satisfy (a) if the integral converges, and typical heat kernel estimates will enable us to decide whether or not (b) holds. Even more than that, good heat kernel estimates will allow us to obtain detailed information about V , such as the rate of

decay at infinity and the rate of blowup as x approaches the singularity y ; information that can then be used to establish conditions (i), (ii) and (iii). This is exactly the strategy we follow in this paper.

Let $K = SG$ denote the Sierpinski gasket, the unique nonempty compact set in the plane satisfying

$$K = \bigcup_{i=0}^2 F_i K \tag{1.3}$$

where $F_i x = \frac{1}{2}(x + q_i)$ and (q_0, q_1, q_2) are the vertices of an equilateral triangle. For any infinite word $w = (w_1, w_2, \dots)$ with $w_j = 0, 1, \text{ or } 2$, define the *blowup* K_∞ as the union of the nested sets

$$K \subseteq F_{w_1}^{-1} K \subseteq F_{w_1}^{-1} F_{w_2}^{-1} K \subseteq \dots \tag{1.4}$$

We will always assume that the blowup is *nondegenerate*, meaning that the blowup word w is not eventually constant. This means K_∞ is noncompact and has no boundary, with a well defined notion of $x \rightarrow \infty$ in K_∞ . Each set $F_{w_1}^{-1} \dots F_{w_m}^{-1} F_{w'_1} \dots F_{w'_k} K$ for any finite word (w'_1, \dots, w'_k) is called a *cell of level $k - m$* , or just a $(k - m)$ -cell. These cells are all similar to K , of Euclidean size $2^{-(k-m)}$, and each cell in K_∞ has three neighboring cells on the same level (thanks to the nondegeneracy assumption). Each cell splits naturally into three cells of one higher level, intersecting at points:

$$F_{w_1}^{-1} \dots F_{w_m}^{-1} F_{w'_1} \dots F_{w'_k} K = \bigcup_{i=0}^2 F_{w_1}^{-1} \dots F_{w_m}^{-1} F_{w'_1} \dots F_{w'_k} F_i K.$$

There is a natural self-similar measure μ on K_∞ that is characterized by $\mu(C) = 3^{-n}$ if C is an n -cell. The blowup K_∞ with measure μ is a fractal analog of the line with Lebesgue measure.

Kigami constructs a self-similar energy \mathcal{E} on K that easily lifts to K_∞ . We can regard \mathcal{E} either as a bilinear $\mathcal{E}(u, v)$ or quadratic $\mathcal{E}(u) = \mathcal{E}(u, u)$ form on a space of functions $\text{dom}\mathcal{E}$ defined by

$$\mathcal{E}(u, v) = \lim_{m \rightarrow \infty} \left(\frac{5}{3}\right)^m \sum_{x \sim_m y} (u(x) - u(y))(v(x) - v(y)) \tag{1.5}$$

where x and y vary over the boundary vertices of all m -cells, and $x \sim_m y$ means x and y are boundary vertices of the same m -cell. In other words, the energy is just a renormalized limit of graph energies on graphs approximating K_∞ . The Laplacian may then be defined by the weak formulation

$$\mathcal{E}(u, v) = \int (-\Delta u)v \, d\mu \text{ for all } v \in \text{dom}\mathcal{E}. \tag{1.6}$$

There is also an equivalent pointwise formula

$$\Delta u(x) = \lim_{m \rightarrow \infty} \frac{3}{2} 5^m \sum_{x \sim_m y} (u(y) - u(x)) \text{ (4 terms in the sum)} \tag{1.7}$$

as a renormalized limit of graph Laplacians.

In terms of the energy, each m -cell has size on the order of $(\frac{3}{5})^m$. We can make this precise in terms of the effective resistance metric, which is discussed in Section 2. Also in this section we discuss heat kernel estimates for the semi-group $e^{t\Delta}$. These are essentially due to Barlow and Perkins [11], using probabilistic methods. When

we pass from K_∞ to a product $(K_\infty)^N$, the heat kernel transforms as a product. In Section 3 we use this observation to estimate the fundamental solution $(-\Delta)^{-1}$ and the resolvent $(I - \Delta)^{-1}$. In particular we show that Coulomb potentials exist when $N \geq 2$, and we prove a relative compactness argument that is valid only for $N = 2$. This sets the stage for Section 4, where we prove the properties (i), (ii), and (iii) for $(K_\infty)^2$, and we find the growth rate for the eigenvalue counting function for negative eigenvalues. In Section 5 we briefly discuss extensions to other self-similar fractals.

The results here are closely related to results on the harmonic oscillator Hamiltonians in [14]. In that context we are able to give more precise information on the potentials, and we work on K_∞ rather than on products.

Notation. We write $A \lesssim B$ to mean that there exists a positive constant c independent of the quantities A and B such that $A \leq cB$. We write $A \approx B$ to mean $A \lesssim B$ and $B \lesssim A$.

2. Heat kernel estimates. Let K_∞ be any nondegenerate infinite blowup of SG. Our goal in this section is to give the heat kernel estimates on K_∞ . First we discuss the resistance metric. Recall the definition

$$R(x, y) = \mathcal{E}(\tilde{u})^{-1} \text{ for } x, y \in \text{SG}, \quad (2.1)$$

where \tilde{u} minimizes $\mathcal{E}(u)$ subject to the conditions $u(x) = 0$ and $u(y) = 1$ (here the energy is over SG). We make the same definition for $x, y \in K_\infty$, with the energy taken over K_∞ . On SG we have the estimate,

$$c_1 \left(\frac{3}{5}\right)^n \leq R(x, y) \leq c_2 \left(\frac{3}{5}\right)^n \quad (2.2)$$

where n is the largest value such that x and y belong to adjacent n -cells. Of course n is positive on SG. We show the same estimates on K_∞ , where now n may be any integer.

Theorem 2.1. *There exist positive constants c_1, c_2 such that (2.2) holds on K_∞ , with n being the largest integer such that x and y belong to adjacent n -cells.*

Proof. Let C and C' be $(n+1)$ -cells containing x and y . Since they are not adjacent, ∂C and $\partial C'$ are disjoint. Define u on V_{n-1} by setting u equal to one on $\partial C'$ and zero elsewhere, and then extending it harmonically. Note that $u(x) = 0$ and $u(y) = 1$ because u is constant on C and C' . Thus $\mathcal{E}(\tilde{u}) \leq \mathcal{E}(u)$. But $\mathcal{E}(u) = 6 \left(\frac{5}{3}\right)^{n-1}$ and this yields the lower bound in (2.2) with $c_1 = \frac{5}{18}$.

For the upper bound we consider the adjacent n -cells C'' and C''' containing x and y , and let $z = C'' \cap C'''$. If $\tilde{u}(z) \geq \frac{1}{2}$ we consider the restriction of \tilde{u} to C'' . Since it takes on values separated by at least $\frac{1}{2}$ on an n -cell, the energy of \tilde{u} on C'' is bounded below by a multiple of $\left(\frac{5}{3}\right)^n$. In particular, this gives a lower bound for the energy of \tilde{u} on K_∞ , hence the upper bound in (2.2). If $\tilde{u}(z) < \frac{1}{2}$ repeat the argument on C''' . \square

The heat kernel estimates on K_∞ have the form

$$h_t(x, y) \approx t^{-\alpha} e^{-c \left(\frac{R(x, y)^\beta}{t}\right)^\gamma} \quad (2.3)$$

for

$$\alpha = \log 3 / \log 5, \beta = \log 5 / \log(5/3), \text{ and } \gamma = \log 2 / \log(5/2) \quad (2.4)$$

and some positive constant c , holding for all $t > 0$. The values of α and β may be interpreted as

$$\alpha = d/(d + 1), \beta = d + 1 \text{ where } d = \log 3/\log(5/3)$$

is the Hausdorff dimension of SG in the resistance metric. (The value γ may be interpreted as $\gamma = 1/(d_w - 1)$ where $d_w = \log 5/\log 2$ is the walk dimension of SG; in fact the value of γ is immaterial in what follows.)

Theorem 2.2. *The estimate (2.3) holds for all $x, y \in K_\infty$ for the heat kernel on K_∞ for all $t > 0$.*

Proof. The result is essentially proved by Barlow and Perkins [11]. We just have to note a couple of minor modifications. The first is that the estimate is proved on the space \tilde{K}_∞ made up of two copies of K_∞ constructed by a constant blowup word and glued at the boundary points. The second is that the estimates are given in terms of the Euclidean distance $|x - y|$. However, when (2.2) holds we have $|x - y| \approx (\frac{1}{2})^n$, so that in fact

$$|x - y| \approx R(x, y)^{\log 2/\log(5/3)}, \tag{2.5}$$

and with this substitution the estimates in [11] are exactly of the form (2.3).

To see that we can transfer the estimates from \tilde{K}_∞ to K_∞ we need the following observation: for any two points $x, y \in K_\infty$ and any bounded neighborhood U containing x and y there exists an isometric neighborhood \tilde{U} in \tilde{K}_∞ with corresponding points \tilde{x}, \tilde{y} (these will vary with the neighborhood U). For our purposes it suffices to take U to be a finite blowup $F_{w_n}^{-1} \circ \dots \circ F_{w_1}^{-1}K$. For n large enough, \tilde{x} and \tilde{y} will be far from the boundary of \tilde{U} , so for fixed t the values $\tilde{h}_{t'}(\tilde{x}, \tilde{q})$ and $\tilde{h}_{t'}(\tilde{y}, \tilde{q})$ for \tilde{q} a boundary point of \tilde{U} and $t' \leq t$ will be substantially smaller than $\tilde{h}_t(\tilde{x}, \tilde{y})$. By probabilistic reasoning, it follows that both the Dirichlet and Neumann heat kernels $\tilde{h}_t^D(\tilde{x}, \tilde{y})$ and $\tilde{h}_t^N(\tilde{x}, \tilde{y})$ will be comparable to $\tilde{h}_t(\tilde{x}, \tilde{y})$ and so satisfy the bounds (2.3). These then transfer to the identical $h_t^D(x, y)$ and $h_t^N(x, y)$ on U . But then $h_t(x, y)$ is the limit of either of these as $n \rightarrow \infty$ and $U \rightarrow K_\infty$, so (2.3) holds for $h_t(x, y)$. \square

3. Resolvent estimates on products. Now consider the product space $(K_\infty)^N$ for $N \geq 2$. Note that by (2.4) we have $\alpha N = \log(3^N)/\log 5 > 1$. The heat kernel on $(K_\infty)^N$ is simply the product

$$h_t^N(x, y) = h_t(x_1, y_1)h_t(x_2, y_2) \cdots h_t(x_N, y_N). \tag{3.1}$$

We extend the metric $R(x, y)$ from K_∞ to $(K_\infty)^N$ by

$$R^N(x, y) = \left(\sum_{j=1}^N R(x_j, y_j)^{\beta\gamma} \right)^{1/\beta\gamma}. \tag{3.2}$$

Then (2.3) extends to

$$h_t^N(x, y) \approx t^{-\alpha N} e^{-c(\frac{R(x,y)^\beta}{t})^\gamma}. \tag{3.3}$$

We obtain a kernel $G^N(x, y)$ for $(-\Delta)^{-1}$ on $(K_\infty)^N$ by integrating the heat kernel

$$G^N(x, y) = \int_0^\infty h_t^N(x, y) dt. \tag{3.4}$$

Using the estimate (3.3) and the change of variable $t \rightarrow tR^N(x, y)^\beta$ we obtain

$$G^N(x, y) \approx R^N(x, y)^{\beta(1-\alpha N)}. \tag{3.5}$$

This uses the fact that the integral

$$\int_0^\infty t^{-\alpha N} e^{-ct^{-\gamma}} dt$$

is finite; near zero the second factor dominates, while near infinity the fact that $\alpha N > 1$ makes the first factor integrable.

Note that the exponent in (3.5) is negative, so $G^N(x, \cdot)$ vanishes at infinity. Since any two fundamental solutions of $-\Delta$ differ by a harmonic function, and a harmonic function vanishing at infinity must be zero by the maximal principle, it follows that (3.4) gives the unique fundamental solution of $-\Delta$ vanishing at infinity.

Similarly, we get a kernel $\mathcal{R}^N(x, y)$ for the resolvent $(I - \Delta)^{-1}$ from the integral

$$\mathcal{R}^N(x, y) = \int_0^\infty e^{-t} h_t^N(x, y) dt. \tag{3.6}$$

Theorem 3.1. *There exists $\delta > 0$ such that*

$$\mathcal{R}^N(x, y) \lesssim R^N(x, y)^{\beta(1-\alpha N)} e^{-cR^N(x, y)^\delta}. \tag{3.7}$$

Proof. By the same argument used to obtain (3.5) we have

$$\mathcal{R}^N(x, y) \lesssim R^N(x, y)^{\beta(1-\alpha N)} \int_0^\infty e^{-tR^N(x, y)^\beta} t^{-\alpha N} e^{-ct^{-\gamma}} dt, \tag{3.8}$$

so it suffices to estimate the integral in (3.8). For $R^N(x, y) \leq 1$ we can drop the first factor, so it suffices to consider the case $R^N(x, y) \geq 1$. We split the integral at $t = R^N(x, y)^{-\beta/2}$. For t below this value we discard the first factor, and the third factor gives us $e^{-cR^N(x, y)^{\beta\gamma/2}}$ and enough decay to make the integral converge. For large values of t we discard the third factor, and the first factor gives us $e^{-\mathcal{R}^N(x, y)^{\beta/2}}$. □

Theorem 3.2. *Let $N = 2$. Then for any $z \in (K_\infty)^2$, the operator $(I - \Delta)^{-1}$ followed by multiplication by $G^2(\cdot, z)$, whose kernel is $K(x, y) = G^2(x, z)\mathcal{R}^2(x, y)$, is a compact operator on $L^2((K_\infty)^2)$.*

Proof. First we observe that $(I - \Delta)^{-1}$ is a bounded operator on $L^2((K_\infty)^2)$ for any N . This is an immediate consequence of spectral theory or (3.6), but it can also be deduced from the estimate (3.7). Let $K_s(x, y) = \chi_s(x)G^2(x, z)\mathcal{R}^2(x, y)$ where χ_s denotes the characteristic function of the ball of radius s about z in the $R(x, y)$ metric. Because $G^2(x, z)$ decays as $x \rightarrow \infty$, it follows that the operator with kernel $K(x, y)$ is the norm limit of the operators with kernel $K_s(x, y)$ as $s \rightarrow \infty$. Since the norm limit of compact operators is compact, it suffices to show that the operators with kernel $K_s(x, y)$ are compact. We will do this by showing that they are of Hilbert-Schmidt class, namely

$$\iint |K_s(x, y)|^2 d\mu(x) d\mu(y) < \infty. \tag{3.9}$$

Now $(K_\infty)^N$ behaves like a space of dimension Nd , for $d = \log 3/\log(5/3)$. In particular

$$\mu(B_s(z)) \lesssim s^{Nd}, \tag{3.10}$$

and $R^N(x, z)^{-a}$ is locally integrable if $a < Nd$. To show the finiteness of (3.9) it suffices to bound $\int |\mathcal{R}^2(x, y)|^2 d\mu(y)$ independently of x , and then to bound

$\int_{B_s(z)} |G^2(x, z)|^2 d\mu(x)$. The second factor on the right in (3.7) controls the integral of $|\mathcal{R}^2(x, y)|^2$ for y away from x , so both estimates require only the local integrability of $R^N(x, y)^{2\beta(1-\alpha N)}$, in other words,

$$2\beta(\alpha N - 1) < Nd \text{ for } N = 2. \tag{3.11}$$

But (3.11) is the same as $N < 2 \log 5 / \log 3$, which is clearly valid for $N = 2$. \square

Note that (3.11) is not valid for $N \geq 3$. So the proof of Theorem 3.2 is only valid for $N = 2$.

4. Spectrum of the hydrogen atom Hamiltonian. Let $H = -\Delta + V$ for $V(x) = -cG^2(x, y)$ on $(K_\infty)^2$ for some fixed $y \in (K_\infty)^2$ and positive constant c .

Theorem 4.1. *H is a self-adjoint operator whose essential spectrum coincides with the essential spectrum of $-\Delta$.*

Proof. Theorem 3.2 says that V is a relatively compact perturbation of $-\Delta$, so the result follows from Weyl’s essential spectrum theorem (Corollary 2 to Theorem XIII.14 in [22]). \square

The essential spectrum of $-\Delta$ on K_∞ is described in Teplyaev [26]. There is a countable set E of eigenvalues of infinite multiplicity (the associated eigenfunctions give an orthonormal basis of $L^2(K_\infty)$). The essential spectrum is the closure of E , which is essentially a Cantor set related to the Julia set of the polynomial $x(5 - x)$. Of course \bar{E} is a subset of $[0, \infty]$, but we also know that $0 \in \bar{E}$, so 0 is the bottom of the essential spectrum. It follows immediately that $-\Delta$ on $(K_\infty)^2$ has pure point spectrum $E + E$ with infinite multiplicity, the essential spectrum is $(\bar{E} + \bar{E})$, and 0 is the bottom of the essential spectrum.

Theorem 4.2. *H is bounded below.*

Remark 1. This follows from a general theorem of Kato and Rellich ([22] Theorem X.12), but verifying the hypotheses of the theorem is not very different from the proof below.

Proof. We use the Sobolev embedding theorem

$$\left(\int_{(K_\infty)^2} (u)^q d\mu \right)^{2/q} \lesssim \mathcal{E}(u) + \|u\|_2^2 \text{ for } q = 4d/(d - 1). \tag{4.1}$$

This is proved in [23] for a 4-fold covering of K^2 , but the same proof works for $(K_\infty)^2$ because we have the same heat kernel estimates. We need to show

$$\langle Hu, u \rangle \geq -b\|u\|_2^2 \text{ for some constant } b, \tag{4.2}$$

which is equivalent to

$$c \int_{(K_\infty)^2} G^2(x, y)|u(x)|^2 d\mu(x) \leq \mathcal{E}(u) + b \int |u|^2 d\mu. \tag{4.3}$$

We apply Hölder’s inequality to the integral on the left side of (4.3), over any ball $B_\varepsilon(y)$, with dual indices p and p' with $p' = q/2 = 2d/(d - 1), p = 2d/(d + 1) = 2 \log 3 / \log 5 > 1$. We obtain

$$\int_{B_\varepsilon(y)} G^2(x, y)|u(x)|^2 d\mu(x) \leq \left(\int_{B_\varepsilon(y)} G^2(x, y)^p \right)^{1/p} \left(\int_{B_\varepsilon(y)} |u|^2 d\mu \right)^{2/q}. \tag{4.4}$$

The first integral on the right side of (4.4) is finite, because the estimate (3.5) dominates the integrand by $R^2(x, y)^{\beta(1-2\alpha)p}$ and $\beta(2\alpha - 1)p = \frac{(d-1)2d}{d+1} < 2d$. By taking ε small enough we may make the integral as small as desired. Using (4.1) we obtain

$$\int_{B_\varepsilon(y)} G^2(x, y)|u(x)|^2 d\mu(x) \leq \delta(\mathcal{E}(u) + \|u\|_2^2). \tag{4.5}$$

But we have the trivial estimate

$$\int_{(K_\infty)^2 \setminus B_\varepsilon(y)} G^2(x, y)|u(x)|^2 d\mu(x) \leq M_\delta \|u\|_2^2 \tag{4.6}$$

where M_δ is the maximum value of $G^2(x, y)$ outside $B_\varepsilon(y)$. Choosing $\delta = 1/c$ and adding (4.5) and (4.6) we obtain (4.3). \square

Again this argument will not work on $(K_\infty)^N$ for $N \geq 3$.

Theorem 4.3. *H has a countable set of eigenfunctions with negative eigenvalues.*

Proof. By a general theorem ([22] Theorem XIII.1) it suffices to show that the max-min formula

$$\lambda_j = \max_{\dim L=j} \min_{u \in L^\perp} \frac{\langle Hu, u \rangle}{\|u\|_2^2} = \min_{\dim L=j+1} \max_{u \in L} \frac{\langle Hu, u \rangle}{\|u\|_2^2} \tag{4.7}$$

yields an infinite number of negative values. This just means that there exist spaces L of arbitrarily large dimension on which the quadratic form $\langle Hu, u \rangle$ is negative, in other words

$$\mathcal{E}(u) < c \int G^2(x, y)|u(x)|^2 d\mu(x). \tag{4.8}$$

This is essentially a dilation argument that requires the potential $G^2(x, y)$ not to decay too rapidly at infinity.

Start with any compactly supported eigenfunction u , so $-\Delta u = \lambda u$ for some fixed λ . Then $\mathcal{E}(u) = \lambda \|u\|_2^2$. If we dilate u by composing with $F_{w_n} \circ F_{w_{m-1}} \circ \dots \circ F_{w_1}$ the resulting function u satisfies $-\Delta u = 5^{-m}\lambda u$, hence $\mathcal{E}(u) = 5^{-m}\lambda \|u\|_2^2$. On the other hand, we have

$$G^2(x, y) \geq c_1 \left(\frac{3}{5}\right)^{m\beta(2\alpha-1)} \tag{4.9}$$

on the support of u , so

$$\int G^2(x, y)|u(x)|^2 d\mu(x) \geq c_1 \left(\frac{3}{5}\right)^{m\beta(2\alpha-1)} \|u\|_2^2.$$

Since $\left(\frac{3}{5}\right)^{\beta(2\alpha-1)} = \frac{5}{9} > \frac{1}{5}$, if we take m large enough we can make (4.8) hold. More generally, we can start with a finite set u_1, u_2, \dots, u_n (for any n) of compactly supported eigenfunctions with disjoint supports and pass to their dilations $\tilde{u}_j = u_j \circ F_{w_m} \circ \dots \circ F_{w_1}$. By the above argument we may take m large enough so that (4.8) holds for each \tilde{u}_j . Since these functions also have disjoint supports it follows that (4.8) holds for their span. \square

With a little more effort, we can estimate the growth rate of the eigenvalue counting function for negative eigenvalues approaching zero. Let

$$N(-\varepsilon) = \#\{\lambda_j \leq -\varepsilon\} \text{ for } \varepsilon > 0. \tag{4.10}$$

Theorem 4.4. $N(-\varepsilon) \approx \varepsilon^{-\delta}$ as $\varepsilon \rightarrow 0$ for

$$\delta = \frac{(\log \frac{25}{9}) \log 9}{(\log \frac{9}{5}) \log 5}.$$

Proof. We start with the known estimate

$$N_1(x) \approx x^\alpha$$

for the eigenvalue counting function on SG with either Dirichlet or Neumann boundary conditions. It follows easily that

$$N_2(x) \approx x^{2\alpha} \tag{4.11}$$

where $N_2(x)$ is the eigenvalue counting function on $SG \times SG$ with either Dirichlet or Neumann boundary conditions.

Next we cut up $(K_\infty)^2$ into a union of cells of varying levels on which V is close to being constant. Say

$$(K_\infty)^2 = \cup C_k \text{ (disjoint except at boundary points),} \tag{4.12}$$

where C_k has level n_k , and let

$$M_k = \sup_{C_k} G^2(\cdot, y) \text{ and } m_k = \inf_{C_k} G^2(\cdot, y). \tag{4.13}$$

We will choose the decomposition (4.12) so that M_k and m_k are of comparable size. Define

$$\begin{cases} V^+ = -cm_k \text{ on } C_k \\ V^- = -cM_k \text{ on } C_k \end{cases} \tag{4.14}$$

so that

$$V^- \leq V \leq V^+, \tag{4.15}$$

and let $H^\pm = -\Delta + V^\pm$. Let \mathcal{D} denote the subspace of $L^2 \cap \text{dom } \mathcal{E}$ of functions vanishing on the boundaries of the cells C_k . Let \mathcal{N} denote the space of L^2 functions with possible discontinuities on the boundaries of the cells C_k with finite energy in each cell C_k . We define

$$\lambda_j^- = \min_{\substack{\dim L=j+1 \\ L \subseteq \mathcal{N}}} \max_{u \in L} \frac{\langle H^- u, u \rangle}{\|u\|_2^2} \tag{4.16}$$

and

$$\lambda_j^+ = \min_{\substack{\dim L=j+1 \\ L \subseteq \mathcal{D}}} \max_{u \in L} \frac{\langle H^+ u, u \rangle}{\|u\|_2^2}. \tag{4.17}$$

It follows easily that

$$\lambda_j^- \leq \lambda_j \leq \lambda_j^+. \tag{4.18}$$

(Note that λ_j^\pm are not eigenvalues of H^\pm). Since the cells C_k behave independently in the definitions of λ_j^\pm , we know that the values λ_j^- are just the union over k of the Neumann eigenvalues of $-\Delta$ on C_k translated by $-cM_k$, so

$$\{\lambda_j^-\} = \{5^{n_k} \mu_i^N - cM_k\} \tag{4.19}$$

where $\{\mu_i^N\}$ are the Neumann eigenvalues of $SG \times SG$. Similarly,

$$\{\lambda_j^+\} = \{5^{n_k} \mu_i^D - cm_k\} \tag{4.20}$$

where $\{\mu_i^D\}$ are the Dirichlet eigenvalues of $SG \times SG$.

Now it follows from (4.18), (4.19) and (4.11) that

$$\begin{aligned} N(-\varepsilon) &\leq \#\{\lambda_j^- \leq \varepsilon\} = \#\{5^{n_k} \mu_i - c M_k \leq -\varepsilon\} \\ &= \sum_k \#\{\mu_i \leq 5^{-n_k}(c M_k - \varepsilon)\} \\ &\lesssim \sum_k 9^{-n_k} (c M_k - \varepsilon)_+^{2\alpha} \end{aligned} \tag{4.21}$$

since $5^\alpha = 3$. Similarly we obtain lower bounds with M_k replaced by m_k . For the decomposition (4.12) we want to take cells C_k of level n_k on which $R(x, y) \approx (\frac{3}{5})^{n_k}$. The exact numbers will depend on the point y , but it is clear that we can always do this so that the number of cells with $n_k = n$ for any $n \in \mathbb{Z}$ is at least one and is bounded above by a universal constant. Note that (3.5) implies

$$m_k \approx M_k \approx \left(\frac{9}{5}\right)^{n_k}. \tag{4.22}$$

Thus we obtain

$$N(-\varepsilon) \approx \sum_{n=-\infty}^{\infty} 9^{-n} \left(c \left(\frac{9}{5}\right)^n - \varepsilon\right)_+^{2\alpha}. \tag{4.23}$$

We can write $\varepsilon = (\frac{5}{9})^r$ for $r = -\log \varepsilon / \log(9/5)$. Then the nonzero contributions to (4.23) correspond to $n \gtrsim -r$. We need to observe that $9 \cdot (\frac{5}{9})^{2\alpha} = 9^{2-(\log 9 / \log 5)} > 1$ to conclude that (4.23) is a geometrically converging series, and

$$N(-\varepsilon) \approx 9^r \cdot \left(\frac{5}{9}\right)^{2\alpha r} = 9^{r(2-(\log 9 / \log 5))} = \varepsilon^{-\delta}.$$

□

5. Other fractals. Consider a more general connected self-similar fractal K in \mathbb{R}^n satisfying

$$K = \bigcup_{i=1}^{N_0} F_i K \tag{5.1}$$

analogous to (1.3), where $\{F_i\}$ are contractive similarities and let K_∞ be an infinite blow-up defined by (1.4). We assume that there is a metric $d(x, y)$ on K , that may or may not be related to the Euclidean distance and a contraction factor ρ such that $d(F_i x, F_i y) \approx \rho d(x, y)$ for all i . (More generally, one would like to allow the factor ρ to depend on i , but we are not able to say anything in this generality.) We assume a separation condition on (5.1) such as the open set condition that allows us to define a self-similar measure μ with

$$\mu(F_w K) = \mu^{|w|} \text{ for } \mu = 1/N_0. \tag{5.2}$$

In particular $\mu(F_i \cap F_j) = 0$ if $i \neq j$. Note that

$$d = \log \mu / \log \rho \tag{5.3}$$

is the Hausdorff dimension of K with respect to the $d(x, y)$ metric and the dimension of the measure μ .

We assume that there exists a self-similar energy form \mathcal{E} on K_∞ (with domain $\text{dom } \mathcal{E}$) satisfying

$$\mathcal{E}(u, v) = \sum_{i=1}^{N_0} \frac{1}{s} \mathcal{E}(u \circ F_i, v \circ F_i) \text{ for } u, v \text{ supported in } K \tag{5.4}$$

and some $s < 1$. We define a Laplacian via the weak formulation

$$\mathcal{E}(u, v) = - \int (\Delta u) v \, d\mu \text{ for all } v \in \text{dom } \mathcal{E}. \tag{5.5}$$

Finally we assume that the heat kernel associated to the Laplacian satisfies the estimate

$$h_t(x, y) \approx t^{-\alpha} e^{-c(\frac{d(x,y)}{t})^\beta} \tag{5.6}$$

for some positive constant α, β, γ . We will discuss below some cases in which all the above assumptions are valid.

The reader should note that there are many different ways that heat kernel estimates appear in the literature. Some of these differences depend on the choice of the metric $d(x, y)$, but others are more arbitrary. In many examples the parameters β and γ are related by $\gamma = \frac{1}{\beta-1}$, so only two parameters appear. One observation we make is that, at least for the results described here, the parameter γ plays no role. Thus it seems unwise to insist on this relationship, which may turn out not to hold in all cases. The parameter β is often interpreted as a “walk dimension”, and so is denoted d_w . The parameter α is often written as $d_s/2$ for d_s interpreted as a “spectral dimension”, but this is predicated on the assumption that the Laplacian is an operator for order 2. This is false for most PCF fractals, and remains to be decided for SC. The factor t^α is sometimes written as $V(x, t^{\frac{1}{\beta}})$, the volume of the ball of radius of radius $t^{\frac{1}{\beta}}$ about x . This is the so-called “Li-Yau” form. Of course, it may or may not be the case that $V(x, t^{\frac{1}{\beta}})$ has a power law growth: this is a statement about dimensionality. Then $\alpha = \frac{d}{\beta}$ for the dimension d . In many cases it is known that $2 \leq d_w \leq 1 + d$, with $d < 2$ if the fractal embeds isometrically in the plane. It is also known that heat kernel estimates are stable under rough isometrics [9]. The reader may consult [1], [2] and [18] for further discussion of heat kernel estimates.

We consider the product space $(K_\infty)^N$ with Laplacian and metric extended as in Section 3. We have the estimate (3.5) holding for the kernel $G^N(x, y)$ of $(-\Delta)^{-1}$, so we need the condition

$$\frac{1}{\alpha} < N \tag{5.7}$$

for the kernel to vanish at infinity, allowing the choice $V(x) = -cG^N(x, y)$ for a Coulomb potential.

Next we consider the analog of Theorem 3.2, which is the key to Theorem 4.2. We do not immediately assume $N = 2$. It is clear that the same argument will work if (3.11) holds, which is equivalent to

$$N < \frac{1}{\alpha - d/2\beta} \tag{5.8}$$

(we are assuming here that $d/2\beta < \alpha$). One set of assumptions that are valid in many examples are the following:

$$\alpha\beta = d \text{ and } \alpha < 1. \tag{5.9}$$

Under these assumptions the conditions on N are just

$$\frac{1}{\alpha} < N < \frac{2}{\alpha}, \tag{5.10}$$

and there is always at least one integer N satisfying them. Note that if $\frac{1}{2} < \alpha < 1$ then $N = 2$ is the only allowable choice, while for $\alpha = \frac{1}{2}$ the only choice is $N = 3$.

Next we consider the analog of Theorem 4.4. (The analog of Theorem 4.3 is also valid.) If we are to have estimates of the form (5.6), we must in fact have

$$\alpha = \frac{\log \mu}{\log(s\mu)}, \quad (5.11)$$

as this follows from (5.4) as in [16] for the growth rate of the eigenvalue counting function on K , $N_1(x) \approx x^\alpha$ (the same α as in (5.6)). Note that $s < 1$ already implies the second condition $\alpha < 1$ in (5.9). We then have

$$N_N(x) \approx x^{N\alpha} \quad (5.12)$$

for the eigenvalue counting function (Dirichlet or Neumann) on K^N . The same reasoning as in the proof of Theorem 4.4 leads to the estimate

$$N(-\varepsilon) \approx \sum_n ((s\mu)^n (c\rho^{n\beta(1-\alpha N)} - \varepsilon)_+)^{N\alpha} \quad (5.13)$$

for the eigenvalue counting function for H on $(K_\infty)^N$. Using (5.11) this is the same as

$$N(-\varepsilon) \approx \sum_n \mu^{nN} (c\rho^{n\beta(1-\alpha N)} - \varepsilon)_+^{N\alpha}, \quad (5.14)$$

the analog of (4.23). We define r so that $\varepsilon = \rho^{-\beta(1-\alpha N)r}$. Then the sum in (5.14) extends from around $n = -r$ (shifted by the constant c in (5.14)) to infinity. We thus need the condition

$$\mu\rho^{\beta(1-\alpha N)\alpha} < 1 \quad (5.15)$$

in order for the right side of (5.14) to be a geometrically convergent series, in which case

$$N(-\varepsilon) \approx (\mu\rho^{\beta(1-\alpha N)\alpha})^{-Nr}. \quad (5.16)$$

Using (5.3) the condition (5.15) is equivalent to

$$d - \alpha\beta(\alpha N - 1) > 0, \quad (5.17)$$

and (5.16) becomes

$$N(-\varepsilon) = \varepsilon^{-\delta} \quad (5.18)$$

for

$$\delta = \left(\frac{d - \alpha\beta(\alpha N - 1)}{\beta(\alpha N - 1)} \right) N \quad (5.19)$$

(note that (5.17) implies $\delta > 0$). In particular, if we assume (5.9), then (5.10) implies (5.17), and (5.19) becomes

$$\delta = \left(\frac{2 - \alpha N}{\alpha N - 1} \right) \alpha N. \quad (5.20)$$

For highly symmetric P.C.F. fractals, such as Lindström's nested fractals, if we take the distance to be the effective resistance metric, the heat kernel estimates (5.6) hold and also (5.9) is valid. Thus both Theorems 4.2 and 4.4 hold, provided N satisfies (5.10), and δ is given by (5.20).

Another type of example is the Sierpinski carpet SC. Here we use the Euclidean distance. Then $\mu = 1/8$, $\rho = 1/3$, so $d = \log 8 / \log 3$. There is a self-similar energy satisfying (5.4) for a value of s numerically approximated as slightly less than .8. The heat kernel estimate (5.6) holds for $\alpha = \log 8 / \log(8/s)$ and $\beta = \log(8/s) / \log 3$, so $\alpha\beta = d$, so (5.9) holds. Since $\frac{1}{2} < \alpha < 1$ in this example, we must take $N = 2$, and (5.20) holds. There are other variants of SC for which similar results hold. See [3]–[8], [10], [15] and [16] for details.

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