DIFFUSION ON DELONE SETS

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Abstract. We consider graphs associated to Delone sets in Euclidean space. Such graphs arise in various ways from tilings. Here, we provide a unified framework. In this context, we study the associated Laplace operators and show Gaussian heat kernel bounds for their semigroups. These results apply to both metric and discrete graphs.

Introduction

In this article we initiate the study of metric graphs associated to Delone sets in arbitrary dimensions.

Delone sets are well-spaced subsets of Euclidean space in the sense that their points have a minimal distance to each other and at the same time do not admit arbitrarily large holes. They have been of interest in geometry for a long time. In recent years they have attracted substantial attention in mathematical physics as they can serve as models for the atomic positions of solids.

In particular, Delone sets (with additional regularity features) play a key role in modeling quasicrystals [Lag, LP]. In this context, both diffraction of Delone sets, see e.g. the survey [BL], and the quantum mechanical treatment of models based on Delone sets are of interest, see e.g. the survey [DEC]. The quantum mechanical treatment is based on the Schroedinger equation. Accordingly, spectral theory of Schroedinger operators i.e. operators of the form Laplacian plus a potential, has been a main topic in the investigation of quasicrystals. While the spectral theory is understood in impressive detail in the one-dimensional case [DEC], this is not the case for the higher dimensional situation. In that case, the operator algebras associated to quasicrystals have been intensively studied, resulting in a deep understanding of their K-theory, see the survey [KP], as well as in investigations centered around an averaged quantity called integrated density of states. Also, some results on generic singular continuous spectra are known [LS] and recent years have witnessed developments in the study of certain product models on lattices, [DCS]. However, as far as the spectral theory of quasicrystal operators in Euclidean space of dimension bigger than one is concerned it seems fair to say that the basic picture is rather unclear. Even the spectral properties of discrete Laplacians alone are not well understood on such basic examples as the Penrose lattice. This may even be seen as one of the most important open questions in this field.

Here, we look at such Laplace type operators from a somewhat different point of view, i.e. from the point of view of diffusion. It turns out that in this respect the situation is much more accessible and the operators are very comparable to the usual Laplacian on Euclidean space. In fact, our main results, Theorem \textsuperscript{6} and Theorem \textsuperscript{7} give Gaussian estimates for rather general classes of operators.
associated to arbitrary Delone sets. This generalizes an earlier result of Telcs \cite{Tel} for the Penrose tiling. At the same time this also generalizes parts of the results of Pang \cite{Pan} on the square lattice. (Note, however, that the main thrust of \cite{Pan} is on scaling of the square lattice, which is not addressed in the present paper.)

The first step in our investigation is to associate graphs to Delone sets. In concrete situations such graphs are already present because there is a tiling structure which either can be seen as a graph structure or gives rise to a graph structure in natural way. To deal with the general situation, we introduce the concept of neighbor relations for an arbitrary Delone set. A pair consisting of a neighbor relation and a Delone set then gives rise to a graph based on the Delone set. In this construction, the well-spacing of Delone sets is reflected in the arising graphs being roughly isometric to $\mathbb{R}^N$, see Corollary \corr{1.8}. All of this is discussed in Section \sect{1}. In Section \sect{2}, we then show that every Delone set admits a canonical neighbor relation. This is based on a study of the Voronoi construction. There, we also discuss how tilings and CW-complexes fit into our framework. From a conceptual point of view Section \sect{1} and Section \sect{2} are rather relevant as they set up the framework to study, which may be of interest for further studies as well, and show how earlier examples fit into the framework.

Our main specific results are then discussed in Section \sect{3} and Section \sect{4}, respectively. More specifically, Section \sect{3} deals with metric graphs and Section \sect{4} deals with discrete graphs. Both metric and discrete graphs can be seen as natural candidates for a study of diffusion on Delone sets. While discrete graphs have - at least implicitly - been around in this context, the above mentioned investigation of the operator algebras and the integrated density of states for metric graphs associated to Delone sets does not seem to have been considered before. This is rather remarkable as metric graphs and their associated operators have attracted attention as models for various kinds of random operators, see e.g. \cite{EKKST, BCFK} for recent collections dealing with metric graphs and their features in a variety of cases. As it stands our results are then the first results on Laplacians on metric graphs associated to aperiodic order. As far as methods go, for both the case of discrete graphs and of metric graphs our main result follows from local regularity features combined with a main theorem from Barlow / Bass / Kumagai \cite{BBK}. In fact, for metric graphs we have to work a bit harder to show the necessary local regularity, which is automatically satisfied in the discrete case.

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1. Delone sets, neighbor relations, and the associated graphs

In this section we introduce the basic objects of our study. Delone sets are subsets of Euclidean space with certain uniform spacing properties. We will associate graphs to Delone sets. The vertices of the graphs will be the points of the Delone sets. The edges will be defined by an additional piece of information. To store this information we introduce the concept of neighbor relations.
Our basic setup is as follows: We consider subsets of Euclidean space $\mathbb{R}^N$. The Euclidean norm is denoted by $\| \cdot \|$ and the closed ball around the origin 0 with radius $S$ is denoted by $B_S$ and the open ball around the origin 0 with radius $S$ by $U_S$. The Euclidean metric on $\mathbb{R}^N$ is denoted by $d$, i.e.

$$d(x, y) := \| x - y \|.$$ 

The closed line segment $[x, y]$ between two points $x, y \in \mathbb{R}^N$ is defined by

$$[x, y] := \{ x + t(y - x) : t \in [0, 1] \}$$

and the open line segment $(x, y]$ between two points $x, y \in \mathbb{R}^N$ is defined by

$$(x, y] := \{ x + t(y - x) : t \in (0, 1) \}.$$  

The Lebesgue measure of a measurable subset of $\mathbb{R}^N$ is denoted by $|M|$ and the cardinality of a set $F$ is denoted by $\#F$.

**Definition 1.1.** Let $\Lambda$ be a subset of $\mathbb{R}^N$. Then, $\Lambda$ is called uniformly discrete if there exists $r > 0$ with

$$\| x - y \| \geq 2r$$

for all $x, y \in \Lambda$ with $x \neq y$. The set $\Lambda$ is called relatively dense if there exists $R > 0$ with

$$\mathbb{R}^N = \bigcup_{x \in \Lambda} (x + B_R).$$

If $\Lambda$ is both uniformly discrete (with parameter $r$) and relatively dense (with parameter $R$) it is called a Delone set or an $(r, R)$-Delone set.

**Remark 1.2.** If $\Lambda$ is uniformly discrete with parameter $r$, then open balls around points of $\Lambda$ with radius $r$ are disjoint. This is the reason for the factor 2 appearing in the above definition. The largest $r$ with this property is called the packing radius of $\Lambda$. On the other hand if $\Lambda$ is relatively dense with parameter $R$, then no point of $\mathbb{R}^N$ has distance larger than $R$ to $\Lambda$. Then, the smallest $R$ with this property is called the covering radius of $\Lambda$.

As mentioned already we need an additional piece of information in order to define graphs.

**Definition 1.3 (Neighbor relation).** A neighbor relation on a Delone set $\Lambda$ is a subset $\mathcal{N}$ of $\Lambda \times \Lambda$ satisfying the following conditions for some $S > 0$:

\begin{enumerate}
  \item[(N0)] $\mathcal{N}$ is symmetric (i.e. $(x, y) \in \mathcal{N}$ if and only if $(y, x) \in \mathcal{N}$) and contains the diagonal $\{(x, x) : x \in \Lambda\}$.
  \item[(N1)] $\| x - y \| \leq S$ for all $(x, y) \in \mathcal{N}$.
  \item[(N2)] For arbitrary $x, y \in \Lambda$ there exists a sequence $(x_0, \ldots, x_n)$ in $\Lambda$ with $x_0 = x$, $x_n = y$ and $(x_i, x_{i+1}) \in \mathcal{N}$, $i = 0, \ldots, n$ and

$$\{x_0, \ldots, x_n\} \subset [x, y] + B_S.$$ 

The number $S$ is called the parameter of the neighbor relation. We write $x \sim y$ if $(x, y) \in \mathcal{N}$ and then say that $x$ and $y$ are neighbors.

**Remark 1.4 (Parameters).** Note that any $(r, R)$-Delone set is an $(r', R')$-Delone set as well for any $0 < r' \leq r$ and $R \leq R'$. Similarly, a neighbor relation to parameter $S$ is a neighbor relation to any parameter $S'$ with $S' > S$. 

Part (N2) of the definition is crucial. It gives a precise way of saying that a point in $\Lambda$ has neighbors in 'all directions'. This will enable us to show that the resulting graphs are roughly isometric to the ambient space. In the next section we will show that any Delone set admits a neighbor relation. More specifically, we will show that

$$N_{\text{max}}(\Lambda) := \{(x, y) \in \Lambda \times \Lambda : \|x - y\| \leq 2R\}$$

is a neighbor relation (with parameter $2R$). By definition this is the maximal neighbor relation to this parameter in the sense that it contains any other such such neighbor relation.

In this section we proceed by developing the theory of neighbor relations and the associated graphs. In particular, we will show how in our setting there is a certain uniformity to all sorts of quantities. Let $\mathcal{N}$ be a neighbor relation on $\Lambda$. We then define for each $x \in \Lambda$ the degree of $x$ as

$$\deg(x) := \#\{y \in \Lambda : y \neq x \text{ and } y \sim x\}.$$ 

**Proposition 1.5** (Uniform bounds). Let $\Lambda$ be an $(r, R)$-Delone set and $\mathcal{N}$ a neighbor relation with parameter $S$ on it.

(a) We have $2r \leq \|x - y\| \leq S$ for all $(x, y) \in \mathcal{N}$ with $x \neq y$.

(b) There is an $D \geq 0$ with $\deg \leq D$.

**Proof.** (a) By $(x, y) \in \mathcal{N} \subset \Lambda \times \Lambda$ we have $2r \leq \|x - y\| \leq S$.

(b) By (a), we can bound $\deg(x)$ by

$$\deg(x) \leq \#(x + BS) \cap \Lambda.$$ 

As $\Lambda$ is an $(r, R)$ Delone set, open balls of radius $r$ around different points of $\Lambda$ are disjoint and we can bound the latter quantity to obtain

$$\#(x + BS) \cap \Lambda \leq \frac{|BS + r|}{|B_r|}.$$ 

This finishes the proof. 

Consider now a pair $(\Lambda, \mathcal{N})$ consisting of an $(r, R)$-Delone set $\Lambda$ and a neighbor relation $\mathcal{N}$. We can then associate a combinatorial graph $G_c(\Lambda, \mathcal{N})$ as follows: The vertices of $G_c(\Lambda, \mathcal{N})$ are given by the elements of $\Lambda$ and the edges of $G_c(\Lambda, \mathcal{N})$ are exactly the pairs $(x, y) \in \mathcal{N}$. Note that the degree of an $x \in \Lambda$ defined above is exactly the degree of the vertex $x$ in the graph $G_c(\Lambda, \mathcal{N})$. In particular, the graph $G_c(\Lambda, \mathcal{N})$ has uniformly bounded degree. For $G_c(\Lambda, \mathcal{N})$ we call a finite sequence $\gamma = (x_0, \ldots, x_n)$ of vertices a path of length $n$ (between $x_0$ and $x_n$) if $x_i \sim x_{i+1}$, $i = 0, \ldots, n$. Then, by (N2), the graph $G_c(\Lambda, \mathcal{N})$ is connected, i.e. between all $x, y \in \Lambda$ there exists a path. As the graph $G_c(\Lambda, \mathcal{N})$ is connected we can define the combinatorial metric $d_c$ on $\Lambda$ by

$$d_c(x, y) := \inf\{n : \text{ there is path of length } n \text{ between } x \text{ and } y\}.$$ 

Finally, the vertex set $\Lambda$ of the graph $G_c(\Lambda, \mathcal{N})$ is naturally equipped with the $\sigma$-algebra of all of its subsets and the canonical measure $\mu_c$ given by

$$\mu_c(S) := \#S$$ 

for $S \subset \Lambda$. In this way $(G_c(\Lambda, \mathcal{N}), d_c, \mu_c)$ is a locally compact, complete metric space with measure $\mu_c$. 
We can also associate to \((A, \mathcal{N})\) the metric graph \(G_m(A, \mathcal{N})\), which arises by ‘gluing’ in intervals between \(x, y \in A\) with \((x, y) \in \mathcal{N}\). Roughly speaking we will glue in the intervals of the form \([x, y]\) and we will consider intervals between different vertices as disjoint. Specifically, we define

\[
G_m(A, \mathcal{N}) := S(A, \mathcal{N}) / \sim,
\]

with

\[
S(A, \mathcal{N}) := \{ (s, (x, y)) \in \mathbb{R}^N \times \mathcal{N} : s \in [x, y] \}
\]

and the relation \(\sim\) given by

\[
(s, (x, y)) \sim (s, (y, x)) \text{ and } (x, (x, z)) \sim (x, (x, z))
\]

for all \((x, y), (x, z) \in \mathcal{N}\) and all \(s \in [x, y]\). The class of an element \((s, (x, y))\) is denoted by \([(s, (x, y))]\).

The elements of the form \([(x, (x, y))]\) are then called the vertices of \(G_m(A, \mathcal{N})\) and the sets

\[
e(x, y) := \{(s, (x, y)) : s \in [x, y]\}
\]

with \((x, y) \in \mathcal{N}\) are called metric edges. The length of the metric edge \(e(x, y)\), denoted by \(l(x, y)\), is defined as

\[
l(x, y) := \|x - y\|.
\]

Note that the metric edge \(e(x, y)\) is canonically homeomorphic and in fact isometrically isomorphic to the open interval \([0, l(x, y)]) in \(\mathbb{R}\). We can introduce a metric on \(G_m(A, \mathcal{N})\) as follows: Let \(a, b \in G_m(A, \mathcal{N})\) be given. Then, a sequence \((x_0, \ldots, x_{n+1})\) of vertices is called an admissible path joining \(a\) and \(b\) if \((x_j, x_{j+1}) \in \mathcal{N}\) for \(j = 0, \ldots, n\) and \(a = [(s, (x_0, x_1))]\) and \(b = [(t, (x_n, x_{n+1})]\) with suitable (unique) \(s, t \in \mathbb{R}^N\). We then define the length of such a path \(l(a, b, x_0, \ldots, x_{n+1})\) as

\[
l(a, b, x_0, \ldots, x_{n+1}) := \|s - x_1\| + \sum_{j=1}^{n-1} |x_j - x_{j+1}| + \|x_n - t\|
\]

and set

\[
d_m(a, b) := \inf l(a, b, x_0, \ldots, x_{n+1}),
\]

where the infimum is taken over all admissible paths joining \(a\) and \(b\). Then, it is not hard to see that \(d_m\) defines a metric on \(G_m(A, \mathcal{N})\). In this way, \(G_m(A, \mathcal{N})\) becomes a metric space. There is a uniform upper bound on the lengths of these metric edges (by the subsequent Lemma 1.7). Note that we also have a uniform lower bound on the lengths of the edges as well as an uniform upper bound on the degree by Proposition 1.5. Given the uniform bounds on the edge lengths and on the degree it is not hard to see that \(G_m(A, \mathcal{N})\) is a complete metric space. Moreover, \(G_m(A, \mathcal{N})\) is locally compact. Clearly, the Lebesgue measure on the edges induces a measure on the graph \(G_m(A, \mathcal{N})\). This measure will be denoted by \(\mu_m\).

**Remark 1.6.** Of course, there is a close relationship between the two graphs \(G_c(A, \mathcal{N})\) and \(G_m(A, \mathcal{N})\). One can think of \(G_c(A, \mathcal{N})\) as a combinatorial graph underlying \(G_m(A, \mathcal{N})\). Conversely, one can think of \(G_m(A, \mathcal{N})\) as arising from \(G_c(A, \mathcal{N})\) by 'gluing in' intervals of length \(l(e)\) at each edge \(e\).
Recall that two metrics \( e \) and \( e' \) on the same space are called equivalent if there exists a \( c > 0 \) with
\[
\frac{1}{c} e' \leq e \leq c e'.
\]

**Lemma 1.7** (Equivalence of distances). Let \( \Lambda \) be a Delone set with neighbor relation \( \mathcal{N} \). The metrics \( d, d_c \) and \( d_m \) are all equivalent on \( \Lambda \).

**Proof.** Chose \( r, R, S > 0 \) such that \( \Lambda \) is an \((r, R)\)-Delone set and \( S \) is a parameter for \( \mathcal{N} \). Let \( x, y \in \Lambda \) be given. Then, we clearly have
\[
d(x, y) \leq d_m(x, y) \quad \text{and} \quad d_m(x, y) \leq S d_c(x, y).
\]

We are now heading to providing an estimate of \( d_c(x, y) \) in terms of \( d(x, y) \). Without loss of generality we assume \( x \neq y \). By (N2), there exists a sequence \( (x_0, \ldots, x_n) \) in \( \Lambda \) with \( x_0 = x, x_n = y \) and \( x_i \sim x_{i+1}, i = 0, \ldots, n \) and
\[
\{x_0, \ldots, x_n\} \subset [x, y] + B_S.
\]

This gives
\[
d_c(x, y) \leq n \leq \Lambda \cap ([x, y] + B_S).
\]

As the open balls with radius \( r \) around different points of \( \Lambda \) are disjoint we can bound the latter term by
\[
... \leq \frac{|[x, y] + B_{S+r}|}{|U_r|}.
\]

To estimate that last term we use that
\[
|[x, y] + B_{S+r}| = \|y - x\| \sigma_N + |B_{S+r}|
\]

with the volume \( \sigma_N \) of the \((S+r)\)-ball in \( \mathbb{R}^{N-1} \). As \( \|y - x\| \geq 2r \) for \( x \neq y \) we find that
\[
|[x, y] + B_{S+r}| \leq \|y - x\| \left( \sigma_N + \frac{1}{2r} |B_{S+r}| \right).
\]

Putting this together we arrive at
\[
d_c(x, y) \leq Cd(x, y)
\]

with
\[
C = \frac{\sigma_N + \frac{1}{2r} |B_{S+r}|}{|B_c|}.
\]

Two metric measure spaces \( (X_j, e_j, \mu_j), j = 1, 2 \) are called roughly isometric if there exists a map \( \phi : X_1 \to X_2 \) as well as \( \rho > 0 \) and \( \delta > 1 \) with
\[
\begin{align*}
\bullet & \quad \bigcup_{x \in X_1} B_{e_2}(\phi(x), \rho) = X_2, \\
\bullet & \quad \frac{1}{\delta}(e_1(x, y) - \rho) \leq e_2(\phi(x), \phi(y)) \leq \delta(e_1(x, y) + \rho) \quad \text{for all } x, y \in X_1, \\
\bullet & \quad \frac{1}{\delta}\mu_1(B_{e_1}(x, \rho)) \leq \mu_2(B_{e_2}(\phi(x), \rho)) \leq \delta\mu_1(B_{e_1}(x, \rho)) \quad \text{for all } x \in X_1,
\end{align*}
\]

where \( B_{e_j}(z, s) \) denotes the ball in \( X_j \) around \( z \) with radius \( s \) with respect to \( e_j \). It is well known that rough isometry is an equivalence relation for metric measure spaces.

**Corollary 1.8** (Rough isometry). The metric measure spaces \((\mathbb{R}^N, d, \lambda), (G_c(\Lambda, \mathcal{N}), d_c, \mu_c)\) and \((G_m(\Lambda, \mathcal{N}), d_m, \mu_m)\) are roughly isometric.

**Proof.** This follows easily from Lemma 1.7. \( \square \)
2. Tiling systems and existence of neighbor relations

In this section we show existence of neighbor relations for arbitrary Delone sets. More specifically, we present two general and canonical ways of associating a neighbor relation to a Delone set. These will be based on the Voronoi construction and the concept of tiling systems. We also show how suitable decompositions of Euclidean space as a CW-complex give rise to a Delone set with a neighbor relation. By the considerations of the previous section we then obtain in all these cases both a combinatorial and a metric graph.

Definition 2.1 (Tiling system). A pair \((\Lambda, (V_x)_{x \in \Lambda})\) consisting of a set \(\Lambda \subset \mathbb{R}^N\) and a family \(V_x, x \in \Lambda\), of compact subsets of \(\mathbb{R}^N\) is called a tiling system with parameters \(r, R > 0\) if the following conditions hold:

- \((x + B_r) \subset V_x \subset (x + B_R)\) for all \(x \in \Lambda\).
- \(\text{int}(V_x) \cap \text{int}(V_y) = \emptyset\) whenever \(x, y \in \Lambda\) with \(x \neq y\). (Here, \(\text{int}\) denotes the interior of a set.)
- \(\bigcup_{x \in \Lambda} V_x = \mathbb{R}^N\).

A set \(V_x\) is referred to as tile with distinguished point \(x\).

By construction the set \(\Lambda\) appearing in the definition of a tiling system with parameters \(r, R > 0\) is an \((r, R)\)-Delone set.

Tiling systems canonically offer the possibility to define neighbor relations:

Example 1 (Canonical neighbor relation). For each tiling system \((\Lambda, (V_x)_{x \in \Lambda})\) we can define a neighbor relation (with parameter \(2R\)) by

\[ N_{\text{can}}(\Lambda, (V_x)_{x \in \Lambda}) := \{ (x, y) \in \Lambda \times \Lambda : V_x \cap V_y \neq \emptyset \} \]

Indeed, \((N0)\) is obviously satisfied and due to \(V_x \subset (x + B_R)\) for any \(x \in \Lambda\) the condition \((N1)\) follows. Finally, one can easily infer \((N2)\) by considering for any \(x, y \in \Lambda\) with \(x \neq y\) the set

\[ \{ z \in \Lambda : V_z \cap [x, y] \neq \emptyset \} \]

Example 2 (Maximal neighbor relation). For each tiling system \((\Lambda, (V_x)_{x \in \Lambda})\) we can define the neighbor relation (with parameter \(2R\))

\[ N_{\text{max}}(\Lambda, (V_x)_{x \in \Lambda}) := \{ (x, y) \in \Lambda \times \Lambda : \|x - y\| \leq 2R \} \]

Clearly, \(N_{\text{max}}(\Lambda, (V_x)_{x \in \Lambda})\) contains the canonical neighbor relation. Thus, it must satisfy \((N2)\) as well. Moreover, it is not hard to see that \((N0)\) and \((N1)\) clearly satisfied. So, \(N_{\text{max}}(\Lambda, (V_x)_{x \in \Lambda})\) is indeed a neighbor relation. It is the maximal neighbor relation with parameter \(2R\) in the sense that any other such neighbor relation must be a subset of it.

Example 3 (Tilings with convex polytopes). If \((\Lambda, (V_x)_{x \in \Lambda})\) is a tiling system where the \(V_x\) are convex polytopes, we can also define the neighbor relation \(N\) to consist of those \((x, y)\) such that \(V_x\) and \(V_y\) share a non-trivial part of an \((N - 1)\)-dimensional surface. It requires some care to show that this is indeed a neighbor relation. A proof can be given as follows: The properties \((N0)\) and \((N1)\) are clear. Thus, it remains to show \((N2)\). Let \(x, y \in \Lambda\) with \(x \neq y\) be given. Then, with \(S_r := B_r \setminus U_r\) the set

\[ U := \{ s \in (x + S_r) : s \in [x, w] \text{ for some } w \in (y + U_r) \} \]
is an open subset of $x + S_r$ and hence a positive surface measure. On the other hand the set

$$N := \{ s \in (x+S_r) : \text{the line through } x \text{ and } s \text{ meets a } k\text{-dimensional surface of } V_z \}$$

has measure zero for any $k \leq N - 2$ and $z \in \Lambda$. Hence, there must exist a $w \in (y + U_r)$ such that $[x, w]$ does not intersect any $k$-dimensional face of $V_z$ for $k \leq (N - 2)$ and $z \in \Lambda$. This rather directly implies (N2).

The previous examples show that a Delone set admitting a tiling system always gives rise to a neighbor relation as well. Next we show that any Delone set appears in a tiling system. This tiling system is defined via the Voronoi construction. As a consequence it is even a tiling system consisting of convex polytopes.

We start with a discussion of the well known Voronoi construction. Let $\Lambda$ be an $(r, R)$-set. To an arbitrary $x \in \Lambda$ we associate the Voronoi cell $V(x, \Lambda) \subset \mathbb{R}^N$ defined by

$$V(x, \Lambda) := \{ p \in \mathbb{R}^N : \| p - x \| \leq \| p - y \| \text{ for all } y \in \Lambda \text{ with } y \neq x \} = \bigcap_{y \in \Lambda, y \neq x} \{ p \in \mathbb{R}^N : \| p - x \| \leq \| p - y \| \}.$$ 

Note that

$$\{ p \in \mathbb{R}^N : \| p - x \| \leq \| p - y \| \}$$

is a half-space. Thus, $V(x, \Lambda)$ is a convex set. Moreover, it is obviously closed and bounded and therefore compact. It turns out that $V(x, \Lambda)$ is already determined by the elements of $\Lambda$ close to $x$. More specifically, we have

$$V(x, \Lambda) = \bigcap_{y \in B(x, 2R)} \{ p \in \mathbb{R}^N : \| p - x \| \leq \| p - y \| \}$$

by Corollary 5.2 in [Se]. This implies that the Voronoi cells are convex polytopes. Moreover, also the following holds.

**Lemma 2.2.** Let $\Lambda$ be an $(r, R)$-set and $x \in \Lambda$ be arbitrary. Then, the following holds.

(a) $V(x, \Lambda)$ is contained in $B(x, R)$.

(b) $V(x, \Lambda)$ contains $B(x, r)$.

**Proof.** (a) This follows from Proposition 5.2 in [Se].

(b) This is immediate from the construction. □

The following proposition is a direct consequence of the preceding lemma.

**Proposition 2.3.** Let $\Lambda$ be an $(r, R)$-set. Then, $(\Lambda, (V_x)_{x \in \Lambda})$ is a tiling system with parameters $r, R$.

By the previous proposition and the example with convex polytopes discussed above, we infer that any Delone set $\Lambda$ comes with a neighbor relation, the Voronoi neighbor relation,

$$\mathcal{N}_V(\Lambda) := \{ (x, y) \in \Lambda \times \Lambda : V_x \text{ and } V_y \text{ share a non-trivial part of an } (N-1)\text{-face} \}.$$ 

Then, also the bigger

$$\mathcal{N}_{\max}(\Lambda) := \{ (x, y) \in \Lambda \times \Lambda : \| x - y \| \leq 2R \}$$

must be a neighbor relation, called the maximal neighbor relation.

We summarize the preceding considerations in the following theorem.
Theorem 4 (Existence of neighbor relations). Let $\Lambda$ be an $(r, R)$-Delone set. Then, both $N_V(\Lambda)$ and $N_{\max}(\Lambda)$ are neighbor relations.

We finish this section by discussing a related but slightly different way of obtaining graphs from Delone sets via suitable $CW$-complexes in Euclidean space.

Example 5 (CW-complexes in Euclidean space). Let a decomposition of $\mathbb{R}^N$ as a $CW$-complex be given such that the following assumptions are satisfied:

(C1) Each cell is a convex polytope.
(C2) There exists a $\rho > 0$ such that each $N$-cell has diameter at most $\rho$.
(C3) There exists an $\gamma > 0$ such that the $k$-dimensional surface measure of any $k$-cell is at least $\gamma$ for $k = 0, \ldots, N$.

Then, the $0$-skeleton $\Lambda$ of this complex is $\gamma/2$ discrete and $\rho$ uniformly dense. Hence, it is a Delone set. We define

$$N := \{(x, y) \in \Lambda \times \Lambda : x, y \text{ belong to the same } 1\text{-dimensional cell}\}.$$ 

Then, $N$ is a neighbor relation with $S = \rho$. Indeed, (N0) is clear and (N1) follows as the length of a 1-cell can not exceed the diameter of any $N$-cell that it belongs to. It remains to show (N2): Let $x, y \in \Lambda$ be given. By (C2) any $N$-cell intersecting $[x, y]$ is contained in $[x, y] + B_\rho$. By construction any two points of the $0$-skeleton belonging to the same $N$-cell are connected. Thus, we infer (N2) with $S = \rho$.

3. Metric graphs over Delone sets and their Laplacians

In this section we discuss the link between metric graphs and the Dirichlet form of an associated Laplacian. We will then also discuss some local regularity features of the Dirichlet forms associated to metric graphs arising from Delone sets. In this discussion we follow [Hae] to which we refer for further details and proofs. We then go on and combine our above considerations with [BBK] to obtain the main result of the paper.

Throughout this section we assume that we are given a Delone set $\Lambda$ with a neighbor relation $N$. We will be concerned with the associated metric graph $(G_m(\Lambda, N), \Lambda)$. In our considerations we will need the Hilbert space $L^2(G_m(\Lambda, N), \mu_m)$ of (equivalence classes of) real valued functions on $G_m(\Lambda, N)$ with inner product

$$\langle u, v \rangle := \int uv d\mu_m.$$

By construction each metric edge is isometrically isomorphic to an open interval in $\mathbb{R}$. In the sequel we will then (tacitly) identify the metric edge with this interval. This will allow us to speak about weak differentiability and weak derivatives of functions (by considering the corresponding functions on the open intervals). In particular, whenever $u$ is a function on $G_m(\Lambda, N)$ which is weakly differentiable on each metric edge we will denote by $u'$ the derivative of $u$. Note that this derivative is not defined on the (countable many) branching points of $G_m(\Lambda, N)$.

By $W^{1, 2}(G_m(\Lambda, N))$ we denote the vector space of all continuous functions $u : G_m(\Lambda, N) \rightarrow \mathbb{R}$ which are weakly differentiable on each metric edge such that

$$\int |u(x)|^2 + |u'(x)|^2 d\mu_m < \infty.$$
When equipped with the inner product
\[
\langle u, v \rangle_{W^{1,2}} := \int u v + u' v' d\mu_m
\]
this becomes a Hilbert space. The energy form associated to \(G_m(\Lambda, \mathcal{N})\) is then given by
\[
\mathcal{D} := \mathcal{D}(\mathcal{E}) = W^{1,2}(G_m(\Lambda, \mathcal{N})), \quad \mathcal{E}(u, v) := \int u' v' d\mu_m(x).
\]
It is not hard to see that this is a closed symmetric form, which is bounded below. The corresponding generator \(\Delta_{\Lambda, \mathcal{N}}\) is known as the Laplacian with Kirchhoff boundary conditions and for a function \(u\) in the operator domain, \(\Delta_{\Lambda, \mathcal{N}} u = -u''\) in a suitable distributional sense, see e.g. [Hae] for further discussion.

The form \(\mathcal{E}\) is a Dirichlet form, i.e. whenever \(u\) belongs to \(\mathcal{D}\) and \(C : \mathbb{R} \to \mathbb{R}\) is a normal contraction (meaning that \(C\) satisfies \(C(0) = 0\) and \(|C(x) - C(y)| \leq |x - y|\) for all \(x, y \in \mathbb{R}\), then \(Cu\) belongs to \(\mathcal{D}\) as well and \(\mathcal{E}(Cu, Cu) \leq \mathcal{E}(u, u)\) holds.

The form has the regularity feature that \(\mathcal{D} \cap C_0(G_m(\Lambda, \mathcal{N}))\) is dense in \(\mathcal{D}\) with respect to the form norm. Indeed, chose an arbitrary function \(\varphi : \mathbb{R} \to [0, \infty)\), which is infinitely many times differentiable, supported in \([-2, 2]\) and equal to 1 in \([-1, 1]\) and define
\[
\phi_n := \varphi(\frac{1}{n} d(p, \cdot))
\]
for a fixed \(p \in G_m(\Lambda, \mathcal{N})\). Then, a simple calculation shows that the \(\phi_n u \in C_0(G_m(\Lambda, \mathcal{N}))\) converge to \(u\) in the form sense for any \(u \in \mathcal{D}\).

Thus, \(\mathcal{E}\) is a regular Dirichlet form. Moreover, \(\mathcal{E}\) is strongly local in the sense that \(\mathcal{E}(u, v) = 0\) whenever \(u\) is constant on the support of \(v\). In fact, the energy measure (which exists by abstract theory for any strongly local Dirichlet form) can easily be seen to be given by
\[
d\Gamma(u(x)) = |u'(x)|^2 d\mu_m(x)
\]
for \(u \in \mathcal{D}\) (cf. [Hae]).

By the discussion in the previous section the graph \(G_m(\Lambda, \mathcal{N})\) has bounded geometry in the sense that the edge lengths are uniformly bounded from below and the vertex degree is uniformly bounded from above. Hence, we can infer from [Hae] the following two local regularity properties, where we denote by \(B_s(x)\) the ball around \(x\) with radius \(s\) with respect to \(d_m\).

**Proposition 3.1** (Uniform local volume doubling). For any \(L > 0\) there exists \(\nu > 0\) such that for all \(x \in G_m(\Lambda, \mathcal{N})\) and all \(s \in (0, L)\) we have
\[
0 < \mu_m(B_{2s}(x)) \leq 2^\nu \cdot \mu_m(B_s(x)) < \infty.
\]

**Proposition 3.2** (Uniform local Poincaré inequality). For any \(L > 0\) there exists \(c\) such that for all \(0 < s < L\) and \(u \in W^{1,2}(B_s(x))\) we have
\[
\int_{B_s(x)} |u(y) - \bar{u}_{B_s(x)}|^2 d\mu_m(y) \leq c L^2 \int_{B_s(x)} |u'(y)|^2 d\mu_m(y).
\]

---

1. By adding points on the edges one can then automatically ensure that the edge lengths are bounded from above as well.
Here, \( \bar{u}_{B_s(x)} \) is the average of \( u \) over \( B_s(x) \) given by

\[
\bar{u}_{B_s(x)} := \frac{1}{\mu_m(B_s(x))} \int_{B_s(x)} u \, d\mu_m.
\]

Let now \( e^{-t \Delta_{A,N}} \), \( t \geq 0 \), be the semigroup which is associated to the operator \( \Delta_{A,N} \). Since \( E \) is a Dirichlet form, this semigroup is Markovian, i.e.

\[
0 \leq e^{-t \Delta_{A,N}} u \leq 1
\]

holds for any \( u \in L^2(G_m(\Lambda,N)) \) with \( 0 \leq u \leq 1 \). Moreover, in [Hae] (see [KLVW] as well) it was shown that this semigroup has a kernel \( p_t : (0, \infty) \times G_m(\Lambda,N) \times G_m(\Lambda,N) \rightarrow (0, \infty) \). Thus, we have

\[
e^{-t \Delta_{A,N}} u(x) = \int p_t(x,y)u(y)d\mu_m(y)
\]

for all \( t > 0 \).

**Theorem 6.** Let \( \Lambda \) be a Delone set in \( \mathbb{R}^N \) with neighbor relation \( N \) and \( G_m(\Lambda,N) \) the associated metric graph. Let \( \Delta_{A,N} \) be the associated Laplacian. Then, there exist \( c_1, c_2, c_3, c_4 > 0 \) such that the kernel \( p \) satisfies

\[
(\text{GE}) \quad c_1 \frac{\exp(-c_2 \frac{d(x,y)^2}{t})}{\mu_m(B_{\sqrt{t}}(x))} \leq p_t(x,y) \leq c_3 \frac{\exp(-c_4 \frac{d(x,y)^2}{t})}{\mu_m(B_{\sqrt{t}}(x))},
\]

for all \( x, y \in G_m(\Lambda,N) \) and \( t > 0 \).

**Proof.** Given the local regularity properties discussed above this follows from stability of corresponding heat kernel estimates under rough isometries as discussed in [BBK]. Here, the basic idea behind this stability is that volume doubling and Poincaré inequality are stable under rough isometries. Now, by results of Sturm [St] volume doubling and Poincaré inequality are equivalent to parabolic Harnack inequality which in turns implies the desired heat kernel estimates. Here are the details for our situation:

We note first that due to Corollary 1.8, the space \( (G_m(\Lambda,N), \mu_m, d_m) \) is roughly isometric to \( (\mathbb{R}^N, \lambda, d) \). It follows from the Propositions 3.1 and 3.2 that the underlying space \( G_m(\Lambda,N) \) satisfies both the uniform local volume doubling property, as well as the uniform local Poincaré inequality. This puts us in the situation, where we can apply Theorem 2.21 (a) from [BBK] with \( X_1 = \mathbb{R}^N \) and \( X_2 = G_m(\Lambda,N) \). Precisely, we deduce from the latter result the full range volume doubling property, as well as the global Poincaré inequality for \( X_2 \). (Note that the statement in [BBK] is stated in higher generality. Our situation corresponds to the case \( \beta_1 = \beta_2 = 2 \).) With this at hand, results from Sturm [St] on strongly local Dirichlet forms conclude the proof. Indeed, noting that closed balls of finite \( d_m \)-radius are compact (hypothesis I(a) in [St]), we have verified all assumptions imposed in the just mentioned paper in order to obtain the desired estimates on the heat kernel. Precisely, the Gaussian upper bound follows from inequality (4.4) in [St] which was derived from Theorem 4.1 of the same paper. The Gaussian lower bound is deduced from Corollary 4.10 in [St]. This finishes the proof. \( \square \)

**Remark 3.3.** The bounds on the heat kernel given in the preceding theorem are known as Gaussian bounds.
• Note that no further regularity conditions on the Delone set are necessary. In particular, even Delone sets arising from corresponding random processes will still satisfy the above Gaussian bounds.
• There is quite some stability to the argument. In fact, the main ingredient is the rough isometry. This will also hold if, for example, the measure $\mu_m$ is replaced by the measure $h\mu$ with a measurable function $h : G_m(\Lambda, N) \to (0, \infty)$ being uniformly bounded away from zero and uniformly bounded from above.
• By applying this result to the metric graph with vertex set $\mathbb{Z}^2$ and edge set $\{(tv+(1-t)w)\mid 0 \leq t \leq 1 \text{ and } v, w \in \mathbb{Z}^2, |v-w| = 1\}$ (which clearly fits into the framework of the example of polytopal tilings) we recover the Gaussian bounds obtained by Pang in [Pan] by means of a completely different method. Note, however, that the main thrust of [Pan] is on the somewhat different issue of scaling.

4. The discrete case

In the preceding sections we have mainly been interested in the case of metric graphs. However, one can also consider the discrete graph associated to a Delone set and a neighbor relation. In this case, one also obtains bounds on the corresponding semigroup by essentially the same methods. This is discussed in this section.

Let $\Lambda$ be a Delone set and $N$ a neighbor relation on $\Lambda$. We consider the Hilbert space $\ell^2(\Lambda) = L^2(\Lambda, \mu_\Lambda)$ consisting of square summable real valued functions on $\Lambda$. The discrete Laplacian $L_{\Lambda, N}$ is the linear operator defined on the whole $\ell^2(\Lambda)$ via

$$L_{\Lambda, N}u(x) := \sum_{y \sim x} (u(x) - u(y)).$$

As the degree is uniformly bounded, this is a bounded operator. It is a non-negative operator with form $\mathcal{E}_c$ given by

$$\mathcal{E}_c(u, v) = \frac{1}{2} \sum_{(x,y) \in N} |u(x) - u(y)|^2.$$

Clearly, this is a Dirichlet form i.e. for any normal contraction $C : \mathbb{R} \to \mathbb{R}$ we have $\mathcal{E}(Cu, Cu) \leq \mathcal{E}(u, u)$. Hence, the associated semigroup $e^{-tL_{\Lambda, N}}$ is Markovian i.e. satisfies $0 \leq e^{-tL_{\Lambda, N}} \leq 1$ whenever $0 \leq u \leq 1$ holds. Since $\Lambda$ is a discrete set, the semigroup has a kernel $p : (0, \infty) \times \Lambda \times \Lambda \to (0, \infty)$.

**Theorem 7.** Let $\Lambda$ be a Delone set in $\mathbb{R}^N$ with neighbor relation $N$ and $G_{\Lambda, N}$ the associated discrete graph. Let $L_{\Lambda, N}$ be the associated Laplacian. Then, there exist $c_1, c_2, c_3, c_4 > 0$ such that the kernel $p$ satisfies

$$c_1 \exp\left(-c_2 \frac{d(x,y)^2}{t}\right) \leq p_t(x, y) \leq c_3 \exp\left(-c_4 \frac{d(x,y)^2}{t}\right),$$

for all $x, y \in G_{c}(\Lambda, N)$ and $t > 1 \vee d_c(x, y)$. 


Proof. As the main result of the previous section, this is essentially a consequence from Theorem 2.21 (and the remark following it) in [BBK]. This time, however, we have to combine this with considerations of Delmotte [Del] and in particular Theorem 3.8 of [Del]. This theorem shows the discrete time version of the estimate (GE). However, the line of argumentation of [Del] carries over to the continuous time case as well. For completeness reasons we next briefly sketch the corresponding argument.

We note that \((\mathbb{R}^N, \lambda, d)\) and \((\Lambda, \mu_c, d_c)\) with are roughly isometric. Since the graph \(G_c(\Lambda, N)\) has uniformly bounded degree all local regularity requirements are automatically satisfied. Indeed, below some fixed scale \(c_0 \geq 1\), local Poincaré inequality always holds for \(G_c(\Lambda, N)\). The argument is the same as the proof of Proposition 5.4 (a) in [BBK]. By Theorem 2.21 (a) of [BBK] applied to \(X_1 = (\mathbb{R}^N, \lambda, d)\) and \(X_2 = G_c(\Lambda, N)\), we obtain that \(G_c(\Lambda, N)\) satisfies volume doubling and Poincaré inequality. The heat kernel estimates then follow from Theorem 3.8 of [Del]. Indeed, the on-diagonal estimates were shown in Proposition 3.1 of [Del]. The Gaussian type upper bound in the space time range \(t > 1 \vee d_c(x, y)\) can be concluded from a combination of Proposition 3.4, (3.18) and the first part of the proof of Theorem 3.8 (applied to the continuous time setting) in [Del]. The corresponding Gaussian type lower bound follows from the on-diagonal lower bound and the volume doubling condition via a chaining argument (e.g. the second part of the proof of Theorem 3.8 in [Del] applied to the continuous time setting). □

Remark 4.1.  
• As in the case of metric graphs, the bounds on the heat kernel given in the preceding theorem are known as Gaussian bounds.
• As the argument is basically the same as in the case of metric graphs, there is, again, quite some stability. For example, we can allow for a weight function
  \[
  b : \mathbb{N} \rightarrow (0, \infty)
  \]
  with \(b(x, y) = b(y, x)\) on the edges provided these weights are uniformly bounded from above and uniformly bounded away from zero. Similarly, we could replace the measure \(m_c\) by any measure \(hm_c\) by any \(h\) which is uniformly bounded away from zero and uniformly bounded from above. The resulting operator then acts by
  \[
  Lu(x) = \frac{1}{h(x)} \sum_{y \sim x} b(x, y)(u(x) - u(y)).
  \]
• As a specific instance of the previous part of the remark, we may chose
  \[
  h : \Lambda \rightarrow (0, \infty), h(x) := |V_x|\]
  and \(b(x, y) := d(x, y)^l\)
  for some \(l \in \mathbb{Z}\), whenever we are given a Delone set \(\Lambda\) (and consider it with the canonical neighbor relation).

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