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Capacity and Quantum Mechanical Tunneling

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Abstract. We connect the notion of capacity of sets in the theory of symmetric Markov process and Dirichlet forms with the notion of tunneling through the boundary of sets in quantum mechanics. In particular we show that for diffusion processes the notion appropriate to a boundary without tunneling is more refined than simply capacity zero. We also discuss several examples in $\mathbb{R}^d$.

1. Introduction

In recent years the theory of symmetric Markov processes has been developed considerably using the connection with the theory of Dirichlet forms, see [1] and references therein. In particular the case of processes over an open set in $\mathbb{R}^d$, given by local generators with singular coefficients (that need not be functions nor generalized functions) has been studied. The usefulness of this approach for quantum theory has been pointed out in [2–5, 29]. It permits the definition of quantum dynamics in situations where the approach via a potential perturbing a kinetic energy term does not work, due to the singularities of the potential or the fact that the potential is neither a measurable nor a generalized function, like in cases of zero range potentials considered in nuclear physics and solid state physics (see e.g. [12–14], and references therein). This is an extension of the usual approach to the definition of Hamiltonian inasmuch as in the cases where the Hamiltonian can be defined as a sum of a kinetic energy term and a not too singular potential, the approach by Dirichlet forms is equivalent with the traditional one [15, 6, 7, 2, 3, 8–10]. Another advantage of the approach to dynamics via Dirichlet forms is the fact that it extends to the case of infinitely many degrees of freedom (see [6, 3, 16] and references therein; see also [17–20]). Moreover it gives an immediate connection with the theory of diffusion processes, the Hamiltonian appearing as the infinitesimal generators of such processes, therefore making available for quantum theory results of this very well studied chapter of modern probability theory. In the other direction this connection suggests developments in the theory of diffusion processes. This connection can be

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seen as a new form of the relation of probabilistic and analytical methods, a sort of development of the original one which schematically could be condensed in the so called Feynman-Kac formula. New questions suggested by the above approach to dynamics have led to a new approach to stochastic equations [4, 1, 21].

To close this opening remark let us recall that the theory of Dirichlet forms and symmetric Markov processes is the natural framework for stochastic mechanics, which in turn is an alternative foundation of quantization (see e.g. [22] and references therein). Among the problems that arise naturally by looking at the mentioned connection between quantum theory and the theory of Dirichlet forms and Markov processes is the one of understanding the behaviour of both the quantum mechanical particle and the associated process at the singularities. This study began in [4] and was pursued in [5], in particular by analyzing to what extent a given process with a singular generator can be approximated by those with smooth generators. As discussed in [4] to the quantum mechanical particle in $\mathbb{R}^d$ is associated a diffusion process. This process can be taken to have state space $\mathbb{R}^d$ ([1], the exceptional polar sets arising first in the construction act as traps from inside and are not hit from outside). Capacity zero sets are not hit by the process. In quantum mechanics on the other hand there is the well-known phenomenon of nontunneling at singularities of the potential. This has been studied in detail in one dimensional models (see e.g. [23–25]). It is quite natural to ask about the connection between nontunneling and capacity zero sets.

It turns out that the relation is more subtle than one might think at first. In fact, roughly speaking, there is no tunneling between two adjacent regions of space if and only if the boundary can be enclosed in the *closure* of a decreasing sequence of open sets of small capacity. This is a much finer condition than the boundary having capacity zero. This paper is dedicated to the detailed analysis of these problems. Note that whereas the one dimensional situation can be analyzed both probabilistically and analytically by Feller's method, in the more dimensional situation such a direct method is not available, and in this case our method clarifies the situation by providing concrete criteria.

In Sect. 2 we define tunneling through the boundary between two adjacent regions of $\mathbb{R}^d$ by the property, roughly speaking, that quantum mechanical transitions are possible between the two regions. This property is put in connection with the direct decomposition of the associated Dirichlet form. A relation with Silverstein's concept of proper invariance [26] is also pointed out.

Section 3 contains the two main results of the paper. First, in the general situation of a regular Dirichlet form, not necessarily local, i.e. not necessarily associated with a diffusion process but only in general with some Hunt process, we give a sufficient condition for the boundary between two adjacent regions of $\mathbb{R}^d$ to have the property of being enclosed in a decreasing sequence of closed sets with small capacity. This property is then shown in the local case, i.e. in the case of a diffusion process, to be a sufficient condition for nontunneling. Conversely if there is nontunneling and the associated process is a diffusion process then the above property regarding the boundary holds.

In Sect. 4 we study several examples. In the one-dimensional case we show how our criteria permit us to study such situations on the line where one has nontunneling or tunneling in relation to the singularities at the origin. A situation when one has nontunneling and yet positive capacity is exhibited. The probabilistic interpretations are also given.

In the more dimensional case we discuss several examples exhibiting a very rich structure of behaviour. Again, examples of tunneling or nontunneling are given.

2. Quadratic Forms and Tunneling

Let $\mathscr{H}$ be a Hilbert space and $\mathscr{H}_1$ be a closed subspace of $\mathscr{H}$ with $\mathscr{H}_1 \neq \{0\}$. Let $\mathscr{H}_2 = \mathscr{H} \ominus \mathscr{H}_1$ be the orthogonal complement of $\mathscr{H}_1$ in $\mathscr{H}$ and let P_i be the orthogonal projection onto $\mathscr{H}_i$, $i=1,2$.

Let $(U_t, t \in \mathbb{R})$ be a one-parameter strongly continuous unitary group acting in $\mathscr{H}$, with infinitesimal generator A so that $U_t = e^{-itA}$. We shall say that U_t is *reduced* by the splitting $\mathscr{H} = \mathscr{H}_1 \oplus \mathscr{H}_2$ iff U_t leaves both $\mathscr{H}_1$ and $\mathscr{H}_2$ invariant, i.e. U_t commutes with the projections P_i, $i=1,2$. Note that the commuting of U_t with P_i for some i already implies that U_t is reduced. It follows from the definition of the infinitesimal generator that U_t is reduced by the above splitting iff A and P_i commute in the sense that $AP_i f = P_i A f$ for all $f \in D(A)$, $i=1,2$. This implies in particular $D(A) = D_1(A) \oplus D_2(A)$ with $D_i(A) \equiv D(A) \cap \mathscr{H}_i$, $i=1,2$. It is also well known that U_t is reduced by the splitting $\mathscr{H} = \mathscr{H}_1 \oplus \mathscr{H}_2$ iff all the spectral projections E_λ^A, $\lambda \in \mathbb{R}$ of A commute with P_i, hence iff any bounded functions of A, defined by the spectral theorem, commute with P_i. Moreover the semigroup $(T_t \equiv e^{-tA}, t>0)$ commutes with P_i iff U_t is reduced.

Now let A be a positive self-adjoint operator in $\mathscr{H}$. We easily see by the spectral theorem that U_t is reduced iff $A^{1/2} P_i f = P_i A^{1/2} f$ for all $f \in D(A^{1/2})$.

There is a well known surjective correspondence between positive self-adjoint operators A on a Hilbert space $\mathscr{H}$ and symmetric bilinear positive closed forms E. The correspondence is given by

$$E(f,g) \equiv (A^{1/2} f, A^{1/2} g),$$

where $(\ ,\ )$ is the scalar product in $\mathscr{H}$ and $E(f,g)$ is the evaluation of the form E at f and g in $D(A^{1/2}) \equiv D(E)$. Let $E_i(f,g) \equiv (A^{1/2} P_i f, A^{1/2} P_i g)$, for all $f, g \in D(A^{1/2} P_i)$.

We shall now prove the following

Lemma 2.1. *The following statements are equivalent:*

1) $U_t \equiv e^{-itA}$ *is reduced by the splitting* $\mathscr{H} = \mathscr{H}_1 \oplus \mathscr{H}_2$.

2) $E = E_1 \oplus E_2$ *in the sense that* $f \in D(A^{1/2})$ *implies* $P_i f \in D(A^{1/2})$ *and*

$$E(f,g) = E_1(f,g) + E_2(f,g)$$

for all $f, g \in D(A^{1/2})$.

Proof. If U_t commutes with P_i, then we saw above that by the spectral theorem $A^{1/2}$ commutes with P_i on $D(A^{1/2})$, in the sense that $A^{1/2} P_i f = P_i A^{1/2} f$ for all $f \in D(A^{1/2})$. Then, for all $f, g \in D(A^{1/2})$

$$\begin{aligned} E(f,g) &= (A^{1/2} f, A^{1/2} g) = (A^{1/2} P_1 f, A^{1/2} P_1 g) \\ &\quad + (A^{1/2} P_1 f, A^{1/2} P_2 g) + (A^{1/2} P_2 f, A^{1/2} P_1 g) \\ &\quad + (A^{1/2} P_2 f, A^{1/2} P_2 g) = E_1(f,g) + E_2(f,g). \end{aligned}$$

Conversely suppose $E(f,g)=E_1(f,g)+E_2(f,g)$ for all $f,g\in D(A^{1/2})$. Note that $f\in D(A)$ and $Af=h$ iff $f\in D(A^{1/2})$ and $E(f,g)=(h,g)$ for any $g\in D(A^{1/2})$. We then see from the assumption that $E(P_1 f,g)=E_1(f,g)=E(f,P_1 g)=(h,P_1 g)=(P_1 h,g)$, which implies $P_1 f\in D(A^{1/2})$ and $AP_1 f=P_1 h=P_1 Af$. □

We shall now consider the special case where $\mathscr{H}=L^2(\Omega,m)$, where Ω is some nonvoid open subset of the d-dimensional Euclidean space $\mathbb{R}^d$ and m is a positive Radon measure on Ω, strictly positive on any non-void open subset of Ω. Let Ω_1 be any m-measurable subset of Ω, and let U_t be a one-parameter group of strongly continuous unitary maps of $L^2(\Omega,dm)$. We shall say that there is *nontunneling* through the boundary $\partial\Omega_1$ (of Ω_1 in Ω) under the action of U_t iff $L^2(\Omega,m)=L^2(\Omega_1,m)\oplus L^2(\Omega-\Omega_1,m)$, and U_t is reduced by the splitting of $L^2(\Omega,m)$. In the following we shall be interested in situations where the quadratic form E is a Dirichlet form in the sense of [1]. Let us first recall the definition of such forms. Let Ω and m be as above. According to [1, Chap. 1.1, p. 5] a *Dirichlet form* on $\mathscr{H}\equiv L^2(\Omega,m)$ is any positive definite symmetric bilinear form E on $\mathscr{H}$ which is densely defined, closed on $\mathscr{H}$ and which has the contraction property $u\in D(E)\Rightarrow E(v,v)\leqq E(u,u)$, with $v\equiv(0\vee u)\wedge 1$. Let A be the unique self-adjoint positive operator A such that $E(f,f)=(A^{1/2}f,A^{1/2}f)$ for all $f\in D(A^{1/2})=D(E)$. By a well-known result (see [1, Chap. 13, Theorem 1.4.1]) $T_t=e^{-tA}$, $t\geqq 0$ is a symmetric Markov semigroup on $L^2(\Omega,m)$ in the sense that T_t is self-adjoint and $0\leqq T_t f\leqq 1$ wherever $0\leqq f\leqq 1$, $f\in L^2(\Omega,m)$. Viceversa any symmetric Markov semigroup T_t on $L^2(\Omega,m)$ comes from a Dirichlet form in the sense that, calling $-A$ its infinitesimal generator so that $T_t=e^{-tA}$, then $(A^{1/2}f,A^{1/2}f)$ is a Dirichlet form.

By the above definitions we have that $U_t=e^{-itA}$ is reduced by a splitting $\mathscr{H}=\mathscr{H}_1\oplus\mathscr{H}_2$ iff T_t commutes with the orthogonal projectors on $\mathscr{H}_i$ and in turn this is equivalent by Lemma 2.1 with the corresponding Dirichlet form $E(f,f)=(A^{1/2}f,A^{1/2}f)$ being reduced by this splitting. Moreover if Ω_1 is an open subset of Ω and there is no tunneling across $\partial\Omega_1$ under the action of U_t, we shall say shortly that there is *nontunneling* (with respect to E, T_t or U_t).

We shall now put our notion of nontunneling in connection with the concept of a proper invariant subset introduced by Silverstein [26, p. 9]. We can extend the Markovian operator T_t on $L^2(\Omega_i,m)$ for any non-negative measurable function f. For a measurable function f, we let $T_t f=T_t f^+ - T_t f^-$ whenever the right hand side makes sense. Then by symmetry and the Markov property T_t is extended to a contraction on $L^P(\Omega,dm)$ for all $1\leqq p\leqq\infty$.

In the definition and discussion of proper invariant sets below we shall use this extension of T_t and denote it again by T_t. According to [26, p. 9] a Borel subset Ω_1 of Ω is said to be *proper invariant* (relative to a given Dirichlet form E or equivalently to a given symmetric Markov semigroup T_t) if $m(\Omega_1)\neq 0$, $m(\Omega-\Omega_1)\neq 0$ and moreover $T_t\chi_{\Omega_1}\leqq\chi_{\Omega_1}$ for all $t>0$, m-a.e. Note that, by the symmetry of T_t, one immediately has that Ω_1 is proper invariant iff $\Omega_2\equiv\Omega-\Omega_1$ is proper invariant. Suppose now E is reduced by the splitting $L^2(\Omega,m)=L^2(\Omega_1,m)\oplus L^2(\Omega_2,m)$. This is equivalent with T_t commuting with the projectors P_i onto $L^2(\Omega_i,m)$ and one can identify P_i with the operator of multiplication by χ_{Ω_i} in $L^2(\Omega,m)$. But $T_tP_i f=P_iT_t f$ for all $f\in L^2(\Omega,m)$ implies the same equation for all m-measurable f such that $0\leqq f\leqq 1$, hence, since $P_iT_t1\leqq P_i1m$-a.e. we have $T_tP_i f1\leqq P_i1m$-a.e., i.e. Ω_1 is proper invariant.

Conversely, suppose now Ω_1 is proper invariant, then $T_t\chi_{\Omega_i} \leqq \chi_{\Omega_i}$, $i=1,2$, m-a.e. Multiplying by χ_{Ω_i} we then get $\chi_{\Omega_1} T_t \chi_{\Omega_2}=0$, $\chi_{\Omega_2} T_t \chi_{\Omega_1}=0$, m-a.e. Since $|\chi_{\Omega_2} T_t \chi_{\Omega_1} f(x)| \leqq \|f\|_\infty \chi_{\Omega_2} T_t \chi_{\Omega_1}(x)=0$ m-a.e. for $f \in L_\infty$, we also see that $\chi_{\Omega_2} T_t \chi_{\Omega_1}=0$ as an operator on $L^2(\Omega_i, m)$.

Similarly we prove $\chi_{\Omega_1} T_t \chi_{\Omega_2}=0$. Then $(\chi_{\Omega_1} T_t - T_t \chi_{\Omega_1})f = \chi_{\Omega_1} T_t \chi_{\Omega_1} f + \chi_{\Omega_1} T_t \chi_{\Omega_2} f - T_t \chi_{\Omega_1} \chi_{\Omega 1} f - T_t \chi_{\Omega_1} \chi_{\Omega_2} f = (\chi_{\Omega_1}-1) T_t \chi_{\Omega 1} f = \chi_{\Omega_2} T_t \chi_{\Omega_1} f = 0$ for all $f \in L^2(\Omega, m)$. This then shows that T_t commutes with P_1, hence also with P_2. Hence we have shown that E is reduced by the splitting iff Ω_1 is proper invariant. Finally we remark that E reduced by the above splitting is equivalent with nontunneling through $\partial\Omega_1$, since χ_{Ω_2} is identified with the projection onto $L^2(\Omega_2, m)$.

We summarize these results in the following:

Lemma 2.2. *Let $\mathscr{H}=L^2(\Omega,m)$, where Ω is an open nonvoid subset of $\mathbb{R}^d$ and m is a positive Radon measure on Ω, strictly positive on any nonvoid open subset of Ω. Let E be a Dirichlet form on $L^2(\Omega,m)$ and let A be the associated positive self adjoint operator so that $E(f,f)=(A^{1/2}f, A^{1/2}f)$, $f \in D(A^{1/2})=D(E)$. Let Ω_1 be an m-measurable subset of Ω, let $\Omega_2 \equiv \Omega - \Omega_1$. Let $\mathscr{H}_i = L^2(\Omega_i, m)$. Then nontunneling across $\partial\Omega_1$ with respect to the splitting $\mathscr{H}=\mathscr{H}_1 \oplus \mathscr{H}_2$ is equivalent to Ω_1 being proper invariant.*

Remark. Silverstein [26, p. 10] calls E irreducible if there are no proper invariant subsets of Ω. A closely related notion is discussed by Faris and Simon [28]. T_t is called indecomposable if there are no Ω_i, $m(\Omega_i) \neq 0$ such that T_t is reduced by the splitting $L^2(\Omega,m)=L^2(\Omega_1,m)\oplus L^2(\Omega_2,m)$. In particular they show that in such a case A cannot have a degenerate ground state.

3. Capacity Zero Sets and Tunneling

Let Ω be an open nonvoid subset of $\mathbb{R}^d$ and let m be a positive Radon measure on Ω, strictly positive on any nonvoid open subset of Ω. Let E be a Dirichlet form on $L^2(\Omega,m)$. E is said to be *regular* if $D(E) \cap C_c(\Omega)$ is dense in $D(E)$ in the $E^{(1)}(f,f) \equiv E(f,f)+(f,f)$ norm and in $C_c(\Omega)$ in supremum norm, where $C_c(\Omega)$ denotes the space of continuous functions of compact support on Ω. Associated with any regular Dirichlet form E there is a notion of *capacity* Cap(B), defined for any subset $B \subset \Omega$. For later use we recall its definition (see [1, Chap. 3.1]). If B is open, define

$$\mathrm{Cap}(B) \equiv \infty \quad \text{if} \quad \mathscr{B}_B \equiv \{u \in D(E) | u \geqq 1 \; m\text{-a.e.} \quad \text{on} \quad B\}$$

is void and $\mathrm{Cap}\, B = \inf_{u \in \mathscr{B}_B} E^{(1)}(u,u)$ if $\mathscr{B}_B \neq \emptyset$. For any $B \subset \Omega$ define Cap(B) $= \inf U$, the infimum being taken over all open subsets U of Ω such that $U \supset B$. It is known that Cap is then a Choquet capacity: for this and other properties of Cap, see Chap. 3.1 of [1].

We denote by ∂B respectively $\bar{B}$ the boundary, respectively the closure of a set $B \subset \Omega$. We have the

Theorem 3.1. *Let Ω be a nonvoid open set in $\mathbb{R}^d$ and m be a positive Radon measure on Ω, strictly positive on any nonvoid open subset of Ω. Let E be a regular Dirichlet* *form on* $L^2(\Omega, m)$. *Consider a nonvoid open subset* Ω_1 *of* Ω *and suppose that* $\chi_{\Omega_1} g \in D(E)$ *for any* $g \in D(E) \cap C_c(\Omega)$. *Then there exists a decreasing sequence* 0_n *of open subsets of* Ω *such that* $\bar{0}_n \supset \partial\Omega_1$ *and* $\mathrm{Cap}(0_n) \to 0$ *as* $n \to \infty$.

Proof. Denote $\partial\Omega_1$ by C and let $C_K = C \cap K$ for any compact set $K \subset \Omega$. Since E is regular, there exists a function $g \in \mathscr{D}(E) \cap C_c(\Omega)$ such that $g=1$ on a neighbourhood U of K. By assumption, $\chi_{\Omega_1} \cdot g$ belongs to $\mathscr{D}(E)$. According to Theorem 3.1.3 of [1]. $\chi_{\Omega_1} \cdot g$ admits a quasi-continuous version h. Namely, there is for any $\varepsilon > 0$ an open set $0_\varepsilon \subset \Omega$ with $\mathrm{Cap}(0_\varepsilon) < \varepsilon$ such that the restriction of h to $\Omega - 0_\varepsilon$ is continuous there and $h = \chi_{\Omega_1} \cdot g$ m-a.e.

Suppose that $C_K \cap (\Omega - \bar{0}_\varepsilon) \equiv \tilde{C}_k$ is nonvoid. Then $V = U \cap (\Omega - \bar{0}_\varepsilon)$ is a neighbourhood of $\tilde{C}_K$ and h is continuous on V. Since $\chi_{\Omega_1} \cdot g$ is identically 1 on an open set $V \cap \Omega_1$ and $h = \chi_{\Omega_1} \cdot g$ m-a.e., $h(x) = 1$ for any $x \in V \cap \Omega_1$. In the same way we see $h(x) = 0$ for any $x \in V \cap (\Omega - \bar{\Omega}_1)$. But this means that h is discontinuous at any point of $\tilde{C}_K$, arriving at contradiction. Therefore $C_K \subset \bar{0}_\varepsilon$.

Let Ω be covered by a countable union of compact sets K_K and let $C_k = C \cap K_k$. Then $C = \bigcup_{k=1}^{\infty} C_k$. For each n and k we can find an open set $0_k^n \subset \Omega$ such that $\mathrm{Cap}(0_k^n) < \frac{1}{2^k}\frac{1}{n}$ and $C_k \subset \bar{0}_k^n$. By the construction above we may assume that 0_k^n is decreasing in n. Then $0_n \equiv \bigcup_{k=1}^{\infty} 0_k^n$ has the desired property $\left(\text{with } \mathrm{Cap}(0_n) < \frac{1}{n}\right)$. □

Remark 1. The assumption in Theorem 3.1 is a necessary condition for nontunneling through $\partial\Omega_1$, by virtue of Lemma 2.1. We shall see conversely that if E is a local regular Dirichlet form in the sense of [1] (see below before Theorem 3.2 for the definition), then the conclusion in Theorem 3.1, coupled with some mild additional condition implies nontunneling though $\partial\Omega_1$.

Remark 2. Any Dirichlet form having $C_c^\infty(\Omega)$ as a core can be written

$$E_0(u,v) \equiv \sum_{i,j=1}^{a} \int_\Omega \frac{\partial u(x)}{\partial x_i}\frac{\partial v(x)}{\partial x_j} v_{ij}(dx)$$

$$+ \iint_{\Omega \times \Omega - D} (u(x)-u(y))(v(x)-v(y)) J(dxdy) + \int_\Omega u(x)v(x)k(dx), \quad (3.1)$$

where $v_{i,j}$, $i,j = 1, \ldots, d$ are Radon measures (not necessarily positive) on Ω such that for any $\lambda \in \mathbb{R}^d$ and any compact set $K \subset \Omega$ one has $\sum_{i,j} \lambda_i \lambda_j v_{ij}(K) \geqq 0$ and $v_{ij}(K) = v_{ji}(K)$. J is a positive symmetric Radon measure on $\Omega \times \Omega - D \equiv \{(x,y) \in \Omega \times \Omega, x \neq y\}$ such that for any compact set K and any open set Ω_0 with $K \subset \Omega_0 \subset \Omega$, one has $\int_{K \times K - D} |x-y|^2 J(dxdy) < \infty$, $J(K, \Omega - \Omega_0) < \infty$. $k(dx)$ is a positive Radon measure on Ω. E_0 is obviously regular (see [1, Theorem 2.2.2]).

Remark 3. It is interesting to notice that the condition $g \in D(E) \cap C_c(\Omega) \Rightarrow \chi_{\Omega_1} g \in D(E)$ of Theorem 3.1 is equivalent with the following seemingly weaker condition, which we call condition R for shortness:

For any point $x_0 \in \partial\Omega_1$ one can find a continuous function $g_{x_0}(\cdot)$ on Ω with $g_{x_0}(x) \neq 0$ for all x in some neighbourhood of x_0 in $\partial\Omega_1$ (with the topology induced on $\partial\Omega_1$ by the one on Ω) and one has $g_{x_0} \in D(E)$ as well as $\chi_{\Omega_1} g_{x_0} \in D(E)$.

Clearly the condition of Theorem 3.1 implies this one, using the regularity of E, as pointed out in the proof of Theorem 3.1. To prove the converse, observe that the functions in $L^\infty(m) \cap D(E)$ form an algebra [1, Theorem 1.4.2]. On the other hand, the condition $g_{x_0} \neq 0$ in a neighbourhood of $x_0 \in \partial\Omega_1$ permits us to construct, using the assumption and the fact that if $u \in D(E)$ then $u \wedge 1 \in D(E)$, functions in $D(E)$ which are equal to χ_{Ω_1} on some open subset of Ω_1 with boundary including a portion of $\partial\Omega_1$ in some compact of Ω.

In the following we shall need to recall a few more notions from the theory of Dirichlet forms and the associated symmetric Markov processes. For any Borel set B with $\mathrm{Cap}(B) < \infty$ we shall denote by e_B the 1-equilibrium potential of B [1, p. 75)]. Then $\mathrm{Cap}(B) = E_1(e_B, e_B)$. We have [1, Theorem 4.3.5, p. 106)] that $P_B^1(x) = E_x(e^{-\sigma B})$ is a quasi-continuous version of e_B, where σ_B is the hitting time of B for the Hunt process ξ_t uniquely (up to equivalence) associated with a regular Dirichlet form E (see [1, Chap. 6, p. 173]), and E_x is the expectation with respect to the process started at $x \in B$. Then $P_B^1(x)$ is the (1 –) hitting probability of B.

We shall now consider local Dirichlet forms. We recall the definition [1, p. 6]. A Dirichlet form E is said to be *local* if $E(u_1, u_2) = 0$ whenever $u_i \in D(E)$, $\mathrm{supp}(u_1 dm) \cap \mathrm{supp}(u_2 dm) = \emptyset$, $\mathrm{supp}(u_i dm)$ compact, $i = 1, 2$. For local Dirichlet forms we have the following

Theorem 3.2. *Let Ω and m be as in Theorem 3.1 and let E be a Dirichlet form on $L^2(\Omega; m)$ which is not only regular but also local. Consider an open subset Ω_1 of Ω and suppose that there is a decreasing sequence of open subsets 0_n of Ω such that $\mathrm{Cap}(0_n) \to 0$ as $n \to \infty$ and $\bar{0}_n \supset \partial\Omega_1 \forall n$. Then if each 0_n separates Ω_1 and $\Omega - \bar{\Omega}_1$ in the sense that any continuous path connecting a point in $\Omega_1 - 0_n$ and $\Omega - \bar{\Omega}_1 - 0_n$ should cross 0_n and if $m(\partial\Omega_1) = 0$, then there is nontunneling through $\partial\Omega_1$.*

Proof. Let ε_n be a sequence decreasing to 0, such that $\mathrm{Cap}(0_n) < \varepsilon_n$. Without loss of generality we can assume the 0_n are decreasing, $\bar{0}_n \supset \partial\Omega_1$, and that $\bigcap_{n=1}^{\infty} \bar{0}_n = \partial\Omega_1$. According to [1, Chap. VI], there exists a diffusion process (a Hunt process with continuous sample paths) $M = (X_t, P_x)$ on Ω associated with the Dirichlet form E. The transition semigroup $P_t f$ of M is a version of the L^2-semigroup $T_t f = \exp(-tA) f$.

Since $\mathrm{Cap}(0_n)$ decreases to 0, we now see in the same way as in the proof of Theorem 4.3.1 of [1] that

$$P_x\left(\lim_{n \to \infty} \sigma_{0_n} = \infty\right) = 1 \quad m\text{-a.e.} \quad x \in \Omega,$$

where σ_{0_n} denotes the hitting time to the set 0_n of the sample paths. Let $x \in \Omega$ and let B be any Borel subset of Ω such that x and B are separated by all the 0_n. By the assumption $\sigma_{0_n} \leqq \sigma_B P_x$-a.e. for any $x \in \Omega_1$, so that we obtain

$$P_x(\sigma_B = \infty) = 1 \quad m\text{-a.e.} \quad x \in \Omega_1,$$

which in turn implies

$$p_t(x,B)=0, \quad \text{i.e.} \quad (e^{-tA}\chi_B)(x)=0 \quad m\text{-a.e.} \quad x\in\Omega_1 .$$

Hence, if $m(\partial\Omega_1)=0$, $T_t\chi_{\Omega_i}=\chi_{\Omega_i}T_t$, proving the nontunneling. q.e.d.

Remark 6. From the proof of Theorem 3.2 we see that the assumption that the 0_n separate Ω_1 and $\Omega-\bar{\Omega}_1$ in Theorem 3.2 can be weakened in the following sense. 0_n may be such that any continuous path connecting Ω_1 and $\Omega-\bar{\Omega}_1$ has to pass *either* through all 0_n or through one of at most countably many disjoint subsets of the boundary, provided each of these subsets has 0 capacity.

Remark 7. In both Theorems 3.1 and 3.2 we can replace everywhere the capacity relative to the Dirichlet form E by the capacity with respect to the part of the Dirichlet form E on any open set V containing $\partial\Omega_1$. For the definition of this concept of part of a Dirichlet form see [1, p. 111]. The reason for the possibility of such a replacement is the same as in the proof of Theorem 4.4.2 in [1, p. 111]. This remark is useful for the estimate of capacities, as we shall see in the next chapter.

Remark 8. Consider the assumptions of Theorem 3.2 without $m(\partial\Omega_1)=0$.

We can divide the points of the boundary $\partial\Omega_1$ into two disjoint Borel subsets U_1, U_2, with $U_1\equiv\partial\Omega_1\bigcap_n 0_n$, $U_2\equiv\bigcup_n(\partial\Omega_1\cap\partial 0_n)$.

Then by the assumption $\mathrm{Cap}(0_n)\to 0$ we have $\mathrm{Cap}(U_1)=0$, hence $m(U_1)=0$. Hence the assumption $m(\partial\Omega_1)=0$ can be replaced by the assumption that $m(U_2)=0$. If we drop this assumption then we can only conclude from the proof that $\chi_{\Omega_1}T_t\chi_{\Omega-\Omega_1-U_1}=\chi_{\Omega_2}T_t\chi_{\Omega-\Omega_2-U_2}=0$, thus the process starting from $x\in\Omega_1$ does not reach $\Omega-\bar{\Omega}_1$ nor the part U_1 of the boundary (but could reach U_2).

4. Some Examples

Let us first consider the 1-dimensional situation where Ω is an interval in $\mathbb{R}$, $\Omega=(0,b)$, $-\infty\leqq a<0<b\leqq\infty$. Let $\Omega_1=(a,0)$, then $\partial\Omega_1=\{0\}$. Let m be a Radon measure on Ω, positive on any open interval. Consider the form

$$E(u,u)=\frac{1}{2}\int_\Omega u'(x)^2\varrho(x)dx, \qquad u\in C_c^\infty(\Omega),$$

where ϱ is a non-negative function on Ω. Suppose that the form E is closable on $L^2(\Omega;m)$. Sufficient conditions for this are given in [1, 4, 27]. Its closure is denoted by E again, it is a particular regular local Dirichlet form and is called an energy form. We let $I_d=(0,d)$ for $0<d<b$.

Lemma 4.1. 1) *If there exists a $b'(<b)$ such that $\varrho(x)\geqq 2Cx^{2\gamma}$, $x\in I_{b'}$, for some positive constants C, γ with $0<\gamma<\frac{1}{2}$, then* $\lim_{d\downarrow 0}\mathrm{Cap}\, I_d>0$.

2) *If there exists a $b'(<b)$ such that $\varrho(x)\leqq 2Cx$, $x\in I_{b'}$, for some positive constants C, then* $\lim_{d\downarrow 0}\mathrm{Cap}(I_d)=0$.

Proof. 1) Denote by Cap_V the capacity associated with the part of E on the interval $V=(a,b')$. According to the proof of [1, Theorem 4.4.2], it suffices to show the assertion for Cap_V (see also Remark 7, Sect. 3). To compute $\mathrm{Cap}_V(K)$ for a compact interval $K \subset V$, we use the following formula (cf. [1, pp. 76]):

$$\mathrm{Cap}_V(K) = \inf_{u \in D_K^V} E_1(u, u),$$

where $D_K^V = \{u \in C_c^\infty(V) : u = 1 \text{ on } K\}$. Take any c, d such that $0 < c < d < b'$. Then, for $K = [c, d]$,

$$\mathrm{Cap}_V(K) \geqq \inf_{u \in D_K^V} C \int_d^{b'} u'^2 x^{2\gamma} dx.$$

The right hand side is attained by the solution u of the Euler equation $(2u' \cdot x^{2\gamma})' = 0$, $u(d) = 1$, $u(b') = 0$, namely, by $u(x) = ((b')^{1-2\gamma} - x^{1-2\gamma})/((b')^{1-2\gamma} - d^{1-2\gamma})$, which gives

$$\mathrm{Cap}_V(K) \geqq \frac{C}{(b')^{1-2\gamma} - d^{1-2\gamma}}.$$

Thus $\mathrm{Cap}_V(I_d) \geqq \mathrm{Cap}_V(K) \geqq C/(b')^{1-2\gamma}$, which is independent of d.

2) Let us compute $\mathrm{Cap}(K)$ for $K = [c, d]$ with $0 < c < d < b'$. Take any c', d' such that $0 < c' < c < d < d' < b'$ and consider the space $L = \{u \in C_c^\infty(c', d') : u = 1 \text{ on } (c, d)$ and $0 \leqq u \leqq 1$ on $(c', d')\}$, then clearly

$$\begin{aligned}\mathrm{Cap}(K) &\leqq \inf_{u \in L} E_1(u, u) \leqq \inf_{u \in L} E(u, u) + m(I_{d'}) \\ &\leqq \inf_{u \in L} C \int_{[c', c] \cup [d, d']} u'^2 x dx + m(I_{d'}).\end{aligned}$$

The infimum is attained by the solution u of the Euler equation $(2u'x)' = 0$, namely by

$$u(x) = \begin{cases} \left(\log \dfrac{c}{c'}\right)^{-1} \log \dfrac{x}{c'}, & c' < x < c \\[2ex] \left(\log \dfrac{d'}{d}\right)^{-1} \log \dfrac{d'}{x}, & d < x < d'. \end{cases}$$

Thus $C^{-1} \cdot \mathrm{Cap}(K) \leqq \left(\log \dfrac{c}{c'}\right)^{-1} + \left(\log \dfrac{d'}{d}\right)^{-1} + m(I_{d'})$. Now letting $c' \downarrow 0$ and setting $d' = 2d (< b')$, $C^{-1} \cdot \mathrm{Cap}(I_d) \leqq (\log 2)^{-1} + m(I_{2d})$, which decreases to zero as $d \downarrow 0$. q.e.d.

Combining this lemma with Theorems 3.1 and 3.2, we immediately get the following:

Theorem 4.1. 1) *If there exists a positive constant C such that the inequality*

$$\varrho(x) \leqq 2C|x|$$

holds either for any $x \in (0, d)$ *for some* $d > 0$ *or for any* $x \in (d, 0)$ *for some* $d < 0$, *and moreover* $m\{0\} = 0$, *then there is nontunneling through* 0.

2) *If there exist positive constants* C, γ *with* $0 < \gamma < \frac{1}{2}$ *such that the inequality*

$$\varrho(x) \geqq 2C|x|^{2\gamma}$$

holds for any $x \in (d_1, d_2)$ *for some* $d_1 < 0 < d_2$, *then there is tunneling through* 0.

Remark 1. According to the Feller classification of the boundary of the one dimensional diffusion, the origin 0 is a regular boundary of $(0, b')$ in the first case of Lemma 4.1, while it is a non-exit boundary in the second case. In fact the local generator of our diffusion is expressed as $\frac{d}{dm}\frac{d}{ds}$ with $ds=\frac{1}{2}\varrho^{-1}dx$.

Hence $s(0,d)$ is finite in the first case of Lemma 4.1 and infinite in the second case, $d>0$. In the particular case $dm=\varrho dx$ we have that if there exists a $b'(<b)$ such that $\varrho(x)=2cx^{2\gamma}$, $x\in I_b$ then 0 is an entrance boundary, a natural boundary if $\gamma=\frac{1}{2}$ (and regular for $\gamma<\frac{1}{2}$).

Remark 2. In the second case of Theorem 4.1, the capacity of the origin 0 is positive. An interesting case arises when the inequality in Theorem 4.1, 1) takes place for positive x, while the inequality in 2) holds for negative x. Then Cap(0) is still positive by virtue of Lemma 4.1, 1), but if $m(\{0\})=0$ then there is nontunneling through 0 by virtue of Theorem 4.1. By the observation made in the proof of Theorem 3.2, we see that the associated diffusion admits no communication between positive real and negative real in this case.

We know (from Remark 1 for instance) that the sample paths in this case can hit the origin from the left but cannot from the right. If the paths could go through 0 from the left, then, by symmetry of the diffusion, they should do so from the right, which is a contradiction. Therefore sample paths arriving at 0 from the left have no way but reflection, at least when the measure m does not charge the boundary.

The preceding method to test tunneling still works for higher dimensional diffusions, to which the one-dimensional methods like Feller's test are no more applicable. Let Ω be a two-dimensional rectangle, $\Omega=(a,b)\times(\alpha,\beta)$, $-\infty\leqq a<0<b\leqq\infty$, $-\infty\leqq\alpha<\beta\leqq\infty$. We let $\Omega_1=(a,0)\times(\alpha,\beta)$. Then $\partial\Omega_1=\{(x,y):x=0, \alpha<y<\beta\}$. Let m be a Radon measure on Ω positive on any nonvoid open set. We consider the form

$$E(u,u)=\frac{1}{2}\int_\Omega (u_x^2+u_y^2)\varrho(x,y)dxdy, \qquad u\in C_c^\infty(\Omega),$$

where ϱ is a non-negative function on Ω. Just as in the one dimensional case, we suppose that the form E is closable on $L^2(\Omega;m)$. Its closure (denoted by E again) is a regular local Dirichlet form.

As before we let $I_d=(0,d)$ for $0<d<b$.

Lemma 4.2. 1) *Assume that there exists a $b'(<b)$ such that*

$$\varrho(x,y)\geqq 2x^{2\gamma}C(y), \qquad x\in I_{b'}, \qquad \alpha<y<\beta,$$

where γ is a constant with $0<\gamma<\frac{1}{2}$ and $C(y)$ is a non-negative function of y with $\int_{\alpha'}^{\beta'} C(y)dy>0$ for any α', β' such that $\alpha<\alpha'<\beta'<\beta$. Then

$$\lim_{d\downarrow 0}\mathrm{Cap}(I_d\times(\alpha',\beta'))>0$$

for any α', β' as above.

2) *Assume that there exists a* $b'(<b)$ *such that*

$$\varrho(x,y) \leqq 2xC(y), \qquad x \in I_{b'}, \qquad \alpha < y < \beta,$$

where $C(y)$ *is a locally integrable non-negative function of* y. *Then*

$$\lim_{d \downarrow 0} \mathrm{Cap}(I_d \times (\alpha', \beta')) = 0$$

for any α', β' *as above.*

Proof. The proof is essentially the same as the proof of Lemma 4.1.

1) Let $V=(0,b')\times(\alpha,\beta)$ and $K=[c,d]\times[\alpha',\beta']$ for $0<c<c'<b'$, $\alpha<\alpha'<\beta'<\beta$. Then

$$\mathrm{Cap}_V(K) \geqq \inf_{u \in D_K^V} \int_{\alpha'}^{\beta'} \left\{ \int_d^{b'} u_x(x,y)^2 x^{2\gamma} dx \right\} C(y) dy.$$

As we saw the proof of Lemma 4.1, 1) the integral in the braces dominates $C/(b')^{1-2\gamma}$ for each $y \in (\alpha', \beta')$, and so we see

$$\mathrm{Cap}_V(I_d \times (\alpha', \beta')) \geqq \frac{1}{(b')^{1-2\gamma}} \int_{\alpha'}^{\beta'} C(y) dy,$$

which is positive independent of $d>0$.

2) Let K be as above and take any c', d', α'', β'' such that $0<c'<c<d<d'<b$ and $\alpha<\alpha''<\alpha'<\beta'<\beta''<\beta$. Choose any function $v \in C_c^\infty(\alpha'', \beta'')$ such that $v=1$ on (α', β') and $0 \leqq v \leqq 1$ on (α'', β'').

Then adopting the same function class L as in the proof of Lemma 1, we see

$$\mathrm{Cap}(K) \leqq \inf_{w=u\otimes v,\, u\in L} E_1(w,w) \leqq \inf_{\substack{w=u\otimes v \\ u\subset L}} \left\{ \left(\int_{[c',c]\cup[d,d']} u'^2 x dx \right) \left(\int_{\alpha''}^{\beta''} v^2 C(y) dy \right) \right.$$
$$\left. + \left(\int_{c'}^{d'} u^2 x dx \right) \left(\int_{\alpha''}^{\beta''} (v')^2 C(y) dy \right) \right\} + m(I_{d'} \times (\alpha'', \beta'')).$$

Thus, setting $M = \sup_{\alpha''<y<\beta''} (v'^2)(y)$, we have

$$\mathrm{Cap}(I_d \times (\alpha'', \beta'')) \leqq (\log 2)^{-1} \int_{\alpha''}^{\beta''} C(y) dy$$
$$+ 2d^2 M \int_{\alpha''}^{\beta''} C(y) dy + m(I_{2d} \times (\alpha'', \beta'')),$$

which decreases to zero as $d \downarrow 0$. q.e.d.

Combining Lemma 4.2 with Theorems 3.1 and 3.2, we arrive at the following:

Theorem 4.2. 1) *If there exists a locally integrable non-negative function* $C(y)$ *of* y *such that the equality*

$$\varrho(x,y) \leqq 2|x| C(y)$$

holds either for any $(x,y)\in(0,d)\times(\alpha,\beta)$ *for some* $d>0$ *or for any* $(x,y)\in(d,0)\times(\alpha,\beta)$ *for some* $d<0$ *and if* $m(\partial\Omega_1)=0$, *then there is nontunneling through* $\partial\Omega_1$.

2) *If there exist a constant* γ *with* $0<\gamma<\frac{1}{2}$ *and a non-negative function* $C(y)$ *of* y *with* $\int_{\alpha'}^{\beta'} C(y)dy>0$ *for any* α', β' $(\alpha<\alpha'<\beta'<\beta)$ *such that the inequality*

$$\varrho(x,y)\geqq 2|x|^{2\gamma}C(y)$$

holds for any $(x,y)\in(d_1,d_2)\times(\alpha,\beta)$ *for some* $d_1<0<d_2$, *then there is tunneling through* $\partial\Omega_1$.

Remark. In Theorem 4.2, 1) we just considered the case where ϱ satisfies the inequalities in a rectangle to one side of the y-axis. However the same result can be obtained e.g. when ϱ satisfies $\varrho(x,y)\leqq 2|x|C(y)$ for all $(x,y)\in(0,d)\times(\delta,\beta)$ and all $(x,y)\in(-d,0)\times(\alpha,\delta)$, for some $\alpha<\delta<\beta$. This corresponds to different situations in Theorem 3.2. Such an example can easily be extended to the case of several rectangles, some at one side and others at the opposite side of the y-axis. Extension to the cases where $\partial\Omega_1$ is a curve are also possible. The extension of Theorem 4.2 to the case of parallelepipeds in $\mathbb{R}^d$ is also immediate.

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