

Average Boundary Conditions in Cauchy Problems*

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We consider the general Cauchy problem with initial data in a Hilbert space and with a formal dissipative linear generator. A complete parametrization is known of the (abstract) boundary conditions which make this problem well set. We exhibit a distinguished subset \mathcal{B}_E of the set \mathcal{B} of boundary conditions and demonstrate explicitly that the evolution associated with each B in \mathcal{B} can be represented as a (time independent) average over the evolutions associated with B' in \mathcal{B}_E . Applications are discussed to Schrödinger equations in bounded regions or with singular potentials.

1. INTRODUCTION

Consider the Cauchy problem

$$(d/dt)f_t = Lf_t, \quad t \geq 0 \tag{1}$$

where the initial data f_0 varies throughout a complex Hilbert space \mathcal{H} (with inner product denoted $\langle \cdot, \cdot \rangle$) and where the linear operator L , with domain $D(L) \subseteq \mathcal{H}$, is dissipative, i.e.,

$$\langle Lf, f \rangle + \langle f, Lf \rangle \leq 0 \quad \text{for all } f \text{ in } D(L).$$

In terms of the evolution operators $U^t, t \geq 0$, defined by the equation $U^t f_0 = f_t$, "solving" (1) means constructing the one parameter contraction semigroup (of evolution operators) with infinitesimal generator L , i.e., constructing the family $\{U^t | t \geq 0\}$ of operators on \mathcal{H} with the properties

- (i) $U^t U^s = U^{t+s}$,
- (ii) $\|U^t\| \leq 1, t \geq 0$,
- (iii) $\|U^t f - f\| \rightarrow 0$ as $t \rightarrow 0^+$,
- (iv) $\|(U^t f - f)/t - Lf\| \rightarrow 0$ as $t \rightarrow 0$, for all f in $D(L)$,

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where $\|\cdot\|$ denotes the norm in \mathcal{H} and also the operator norm for bounded operators on \mathcal{H} .

Now the above problem is well set only if there is a *unique* solution f_t of (1) for each f_0 , and $t > 0$. However if L were, for example, a differential operator on a bounded region in \mathbf{R}^n , we would expect to have to choose from a variety of "auxiliary conditions" (traditionally *boundary* conditions) in order to uniquely specify the evolution.

Treating the abstract problem (1), Phillips has given in [1] a complete classification of all possible (abstract) auxiliary conditions (and therefore of their associated infinitesimal generators and evolution semigroups) for each of two situations of very general interest; where one requires the actual infinitesimal generator L to be either (a) an *extension* of a given "minimal operator" L_{\min} , or (b) a *restriction* of a given "maximal operator" L_{\max} . We will parametrize such extensions and restrictions by $B \in \mathcal{B}$.

As an example consider $\mathcal{H} = L_2(0, 1)$ and $L_{\min} = d/dx$ with $D(L_{\min})$ the infinitely differentiable functions with compact support in the open interval $(0, 1)$. It is an easy exercise to show that the set of all contraction semigroups whose generators extend L_{\min} can be parametrized by $\mathcal{B} = \{z \in \mathbf{C} \mid |z| \leq 1\}$ where

$$(U_z^t f)(x) = z^{\lfloor x+t \rfloor} f(\lfloor x+t \rfloor_F) \quad (2)$$

and $\lfloor y \rfloor_I$ (resp. $\lfloor y \rfloor_F$) denotes the integral part (resp. fractional part) of y . Note that U_z^t is invertible (i.e., unitary) if and only if $|z| = 1$.

In this paper, for each of the cases (a) and (b) we will topologize the parameter space \mathcal{B} , exhibit a *distinguished subset* \mathcal{B}_E of \mathcal{B} and then construct, for each B in \mathcal{B} , a regular Borel probability measure μ_B on \mathcal{B} , *concentrated on* \mathcal{B}_E , with the property that

$$U_B^t = \int U_{B'}^t d\mu_B(B') \quad \text{for all } t \geq 0.$$

In terms of (2) for example, $\mathcal{B}_E = \{z \in \mathcal{B} \mid |z| = 1\}$, and if $z = r \exp(i\theta)$, $0 \leq r \leq 1$, and $z' = \exp(i\theta')$, then

$$\begin{aligned} U_z^t &= \int U_{z'}^t d\mu_z(z') = \frac{1}{2\pi} \int_0^{2\pi} U_{z'(\omega)}^t d\varphi \\ &= \frac{1}{2\pi} \int_0^{2\pi} U_{\exp[i\varphi(\theta')]}^t \left[\frac{1-r^2}{|\exp(i\theta') + r|^2} \right] d\theta' \end{aligned}$$

where $\exp[i\varphi(\theta')] = \exp[i(\theta - \theta')][\exp(i\theta') + r]/[\exp(-i\theta') + r]$.

The fact that in this example the general noninvertible (i.e., time irreversible) evolution is represented as an average over invertible (i.e., time reversible) evolutions will be seen to be a consequence of the fact that $KL_zK = L_z^*$ (where $*$ denotes operator adjoint) for each of the infinitesimal generators L_z , where \overline{K} is a conjugation operator on \mathcal{H} (in this example $(Kf)(x) = \overline{f(1-x)}$.) Of course the average of distinguished semigroups with respect to a probability measure is not in general a semigroup. In this example, only the special measures μ_z give rise to semigroups.

Finally, connection is made with the work of Nelson [2] on Schrödinger equations with singular potentials.

2. NOTATION

Throughout this paper \mathcal{H} will denote a fixed separable complex Hilbert space of dimension ≥ 1 and I will denote the identity operator on \mathcal{H} . Given complex Hilbert spaces X and Y (of dimension ≥ 1), $\mathcal{B}(X, Y)$ will denote the Banach space of continuous linear maps from X into Y , with open (resp. closed) ball $\mathcal{B}_r(X, Y)$ (resp. $\overline{\mathcal{B}}_r(X, Y)$) of radius r . Unless otherwise indicated $\mathcal{B}(X, Y)$ and its subsets will be assumed to be in the strong operator topology. If X_1 is a proper nonzero subspace of X and Y_1 is a nonzero subspace of Y , an element of $\mathcal{B}(X_1, Y_1)$ will often be identified, without comment or notational distinction, with its unique extension in $\mathcal{B}(X, Y)$ whose kernel contains $X_1^\perp = X \ominus X_1$ (the orthogonal complement in X of X_1). $\mathcal{B}(X, X)$ will be written $\mathcal{B}(X)$, P_X denotes the orthogonal projection on X_1 , and $\mathcal{B}_E(X, Y)$ is defined to be the set $\{V \in \mathcal{B}(X, Y) \mid V^*V = P_X \text{ or } VV^* = P_Y \text{ or both}\}$, which is always nonempty. Note that $\mathcal{B}_E(X, Y)$ is the set of extreme points of the convex set $\overline{\mathcal{B}}_1(X, Y)$.

3. CALCULATION OF A CHOQUET BOUNDARY

Given B in $\overline{\mathcal{B}}_1(X, Y)$, where X and Y are nonzero subspaces of \mathcal{H} , consider the polar decomposition $B = UR$, where U in $\mathcal{B}(X, Y)$ is a partial isometry and $R = (B^*B)^{1/2}$ in $\mathcal{B}(X)$ satisfies $0 \leq R \leq P_X$. For z in \mathbf{C} , $|z| \leq 1$, we define $R(z)$ in $\mathcal{B}(X)$, by the functional calculus in R , as $f_z(R)$ where f_z is the following function on $[0, 1]$:

$$\begin{aligned}
 f_z(\lambda) &= \frac{z + \lambda}{1 + z\lambda}, & z \neq -1, & \quad 0 \leq \lambda \leq 1, \\
 &= -1, & z = -1, & \quad 0 \leq \lambda < 1, \\
 &= 1, & z = -1, & \quad \lambda = 1.
 \end{aligned}$$

Note that $R(z)$ is norm analytic in z for $|z| < 1$ and (strong operator) continuous in z for $|z| \leq 1$. (The former is a standard fact in operator theory [3, 4.3.1] and the latter follows easily using Lebesgue's dominated convergence theorem.) Furthermore, if $|z| = 1$, it is clear that $R(z)$ is unitary in $\mathcal{B}(X)$. Now if $U \notin \mathcal{B}_E(X, Y)$, i.e., $U^*U = P_F$ and $UU^* = P_G$ with $F \neq X$ and $G \neq Y$, choose any V in $\mathcal{B}_E(F^\perp, G^\perp)$ and define, for $|z| \leq 1$, $B(z) = UR(z) + zV$ and $B_n(z) = (1 - (1/n))B(z)$, $n = 1, 2, \dots$. If $U \in \mathcal{B}_E(X, Y)$, define, for $|z| \leq 1$, $B(z) = B$ and $B_n(z) = (1 - (1/n))B$, $n = 1, 2, \dots$. Then for any B in $\mathcal{B}_1(X, Y)$, $B(0) = B$, while if $|z| = 1$, $B(z) \in \mathcal{B}_E(X, Y)$. Let $F(X, Y)$ be the algebra of those continuous functions f from $\mathcal{B}_1(X, Y)$ into $\mathcal{B}(\mathcal{H})$ which are Gâteaux differentiable on $\mathcal{B}_1(X, Y)$ (i.e., $[f(A + zB)h - f(A)h]/z$ is Cauchy as $z \rightarrow 0$, for $A, B \in \mathcal{B}_1(X, Y)$ and $h \in \mathcal{H}$), and bounded in the sense that the range of f is contained in $\mathcal{B}_r(\mathcal{H})$ for some radius r (which may depend on f). We note using [3, 3.17.1] that such f are automatically Fréchet differentiable on $\mathcal{B}_1(X, Y)$, i.e., $[f(A + B)h - f(A)h]/\|B\|$ is Cauchy as $\|B\| \rightarrow 0$, for $A, B \in \mathcal{B}_1(X, Y)$, and $h \in \mathcal{H}$. If $f \in F(X, Y)$ and $B \in \mathcal{B}_1(X, Y)$, then $f[B(z)] = \lim_{n \rightarrow \infty} f[B_n(z)]$ is continuous in z for $|z| \leq 1$ and, by Vitali's theorem [3, 3.14.1], differentiable in z for $|z| < 1$. Therefore by Cauchy's integral formula [3, 3.11.3], if Γ is the unit circle in \mathbf{C} ,

$$f(B) = f[B(0)] = \frac{1}{2\pi i} \int_{\Gamma} \frac{f[B(z)]}{z} dz = \frac{1}{2\pi} \int_0^{2\pi} f[B(\exp(i\theta))] d\theta. \quad (3)$$

Define $\mathcal{B}_B = \{B[\exp(i\theta)] \mid 0 \leq \theta \leq 2\pi\}$. Formula (3) is our main technical tool; we summarize the above argument in

LEMMA 1. *For each B in $\mathcal{B}_1(X, Y)$, Eq. (3) explicitly defines a regular Borel probability measure, μ_B , on $\mathcal{B}_B(X, Y)$, concentrated on $\mathcal{B}_B \subseteq \mathcal{B}_E(X, Y)$ and such that for all f in $F(X, Y)$*

$$f(B) = \int f(B') d\mu_B(B').$$

Remark. Each \mathcal{B}_B is compact and therefore Borel measurable, and μ_B is concentrated on \mathcal{B}_B in the sense that (by definition) $\mu_B(S) = \mu_B(S \cap \mathcal{B}_B)$ for every Borel measurable S .

Remark. Since $\mathcal{B}_E(X, Y)$ is the set of convex extreme points of $\bar{\mathcal{B}}_1(X, Y)$, and since the identity function is in $F(X, Y)$, $\mathcal{B}_E(X, Y)$ is the smallest subset of $\bar{\mathcal{B}}_1(X, Y)$ which can play the desired role in Lemma 1; thus $\mathcal{B}_E(X, Y)$ is the Choquet boundary of $F(X, Y)$.

4. PHILLIPS' CLASSIFICATION

With any operator L on \mathcal{H} which is dissipative, we can associate the Cayley transform $J = (I + L)(I - L)^{-1}$ with domain $D(J) = \text{Ran}(I - L)$. Conversely, with any contraction J on \mathcal{H} , with domain $D(J)$, such that $\text{Ran}(I + J)$ is dense in \mathcal{H} , we can associate the operator $L = (J - I)(J + I)^{-1}$ with $D(L) = \text{Ran}(I + J)$. These facts are discussed by Phillips in [1] where he proves the two theorems:

THEOREM P_1 . *If L is a dissipative operator with dense domain in \mathcal{H} , then its Cayley transform J is a contraction operator and $\text{Ran}(I + J)$ is dense; L and J are closed together. Conversely, if J is a contraction operator with $\text{Ran}(I + J)$ dense in \mathcal{H} , the associated operator L is a dissipative operator with dense domain and J is its Cayley transform. The pairing $J \leftrightarrow L$ is a one-to-one inclusion preserving correspondence between all dissipative extensions \tilde{L} of L and all contraction extensions \tilde{J} of J . In particular the maximal dissipative extensions \tilde{L} of L correspond to the contraction extensions \tilde{J} of J with $D(\tilde{J}) = \mathcal{H}$.*

THEOREM P_2 . *An operator \tilde{L} is the infinitesimal generator of a contraction semigroup on \mathcal{H} if and only if \tilde{L} is a maximal dissipative operator with dense domain.*

Before we continue it will be convenient to reparametrize the above classification by means of a simple geometric lemma, which we will prove by a variation of the proof of the polar decomposition. From here on L will always denote a fixed closed dissipative operator with dense domain $D(L) \subseteq \mathcal{H}$, J will be its Cayley transform with closed domain denoted M , and we will be describing features of those extensions \tilde{J} of J such that the associated \tilde{L} generates a contraction semigroup, i.e., the contraction extensions \tilde{J} of J with $D(\tilde{J}) = \mathcal{H}$.

Since J is in $\bar{\mathcal{B}}_1(M, \mathcal{H})$, \bar{J} in $\bar{\mathcal{B}}_1(\mathcal{H})$ extends J if and only if $\bar{J} = J + V$ where $V \in \bar{\mathcal{B}}_1(M^\perp, \mathcal{H})$ and $\|\bar{J}^*\| \leq 1$. The last condition is equivalent to

$$\|J^*f\|^2 + \|V^*f\|^2 \leq \|f\|^2 \quad \text{for all } f \text{ in } \mathcal{H}, \text{ i.e., } VV^* \leq I - JJ^*. \quad (4)$$

Let \mathcal{V} denote the set of all V in $\bar{\mathcal{B}}_1(M^\perp, \mathcal{H})$ satisfying (4). Note that if V is any operator of the form $V = (I - JJ^*)^{1/2}B$ where $B \in \bar{\mathcal{B}}_1(M^\perp, \bar{N})$ and \bar{N} is the closure of $N \equiv \text{Ran}(I - JJ^*)$, then

$$\|V^*f\|^2 = \|B^*(I - JJ^*)^{1/2}f\|^2 \leq \|(I - JJ^*)^{1/2}f\|^2$$

for all f in \mathcal{H} , so V is in \mathcal{V} . On the other hand, if V is in \mathcal{V} , define the operator T on \mathcal{H} , with dense domain the linear span of N and N^\perp , by

$$T = V^*(I - JJ^*)^{-1/2} P_{\bar{N}}.$$

Note using (4) that for f in $D(T)$,

$$\begin{aligned} \|Tf\|^2 &= \langle (I - JJ^*)^{-1/2} P_{\bar{N}}f, VV^*(I - JJ^*)^{-1/2} P_{\bar{N}}f \rangle \\ &\leq \langle (I - JJ^*)^{-1/2} P_{\bar{N}}f, (I - JJ^*)(I - JJ^*)^{-1/2} P_{\bar{N}}f \rangle \\ &\leq \|f\|^2 \end{aligned}$$

so $\|\bar{T}\| \leq 1$ where $\bar{T} \in \bar{\mathcal{B}}_1(\mathcal{H})$ denotes the closure of T . Let $B = (\bar{T})^*$. Then for f in N ,

$$B^*(I - JJ^*)^{1/2}f = V^*(I - JJ^*)^{-1/2} P_{\bar{N}}(I - JJ^*)^{1/2}f = V^*f$$

and for f in N^\perp ,

$$B^*(I - JJ^*)^{1/2}f = 0 = V^*f$$

so $V = (I - JJ^*)^{1/2}B$. Now $\|B\| \leq 1$ and $B^*P_{N^\perp} = 0$, so $BB^* \leq P_{\bar{N}}$. Also $BP_M = 0$, so $B^*B \leq P_{M^\perp}$, and therefore $B \in \bar{\mathcal{B}}_1(M^\perp, \bar{N})$. We have thus proven

LEMMA 2. *The contraction extensions \bar{J} of J with domain \mathcal{H} are uniquely represented in the form $\bar{J} = J + (I - JJ^*)^{1/2}B$, where B varies throughout $\bar{\mathcal{B}}_1(M^\perp, \bar{N})$.*

5. EXTREME SEMIGROUPS AND THE REPRESENTATION THEOREMS

Using Theorems P_1 and P_2 , and Lemma 2, we may parametrize the set of operators \bar{L} which extend L and generate contraction semigroups, by the elements B of $\bar{\mathcal{B}}_1(M^\perp, \bar{N})$; the infinitesimal

generator corresponding to B will be denoted L_B , with Cayley transform J_B and associated semigroup $\{U_B^t \mid t \geq 0\}$.

DEFINITION. Those infinitesimal generators L_B , and associated J_B and $\{U_B^t \mid t \geq 0\}$, which correspond to B 's in $\mathcal{B}_E(M^\perp, \bar{N})$, will be called *extreme*.

Note that for $\lambda \in \mathbf{C}$ with $\text{Re } \lambda > 0$, $R(\lambda, B) = (\lambda I - L_B)^{-1}$ is the resolvent of L_B , and that $R(1, B) = (I + J_B)/2$. For $|\lambda - 1| < 1$, a well-known argument [3, 5.8.4] yields

$$R(\lambda, B) = \sum_{n=1}^{\infty} (\lambda - 1)^{n-1} [R(1, B)]^n \tag{5}$$

so that $R(\lambda, B)$ is the limit of Gâteaux differentiable functions from $\mathcal{B}_1(M^\perp, \bar{N})$ into $\mathcal{B}(\mathcal{H})$, and therefore also has this property [3, 3.18.1]; therefore $[R(\lambda, B)]^m$ does also, for $m = 1, 2, \dots$. By iteration, this argument extends to all $\lambda \in \mathbf{C}$ with $\text{Re } \lambda > 0$. From [3, 11.6.6],

$$U_B^t = \lim_{n \rightarrow \infty} [(n/t) R((n/t), B)]^n, \quad t > 0$$

and therefore (using [3, 12.3.2 and 3.18.1]) U_B^t is also Gâteaux differentiable on $\mathcal{B}_1(M^\perp, \bar{N})$ for fixed $t \geq 0$. Finally, from [4, Theorem 2.16] we see that for fixed $t \geq 0$, U_B^t is continuous on $\mathcal{B}_1(M^\perp, \bar{N})$ and is therefore in $F(M^\perp, \bar{N})$. Using Lemma 1 and Theorems P_1 and P_2 , we have proven

THEOREM 1. *If L is a densely defined dissipative operator on \mathcal{H} , every contraction semigroup $\{U_B^t \mid t \geq 0\}$ which is generated by an extension L_B of L can be represented in the form*

$$U_B^t = \int U_{B'}^t d\mu_B(B'), \quad t \geq 0 \tag{6}$$

where μ_B is a regular Borel probability measure concentrated on the extreme semigroups (and independent of t).

The related problem where one seeks an infinitesimal generator which is the restriction of a given operator, is easily treated using the above analysis together with another result of Phillips [1],

THEOREM P_3 . *The operator L on \mathcal{H} is the infinitesimal generator of the contraction semigroup $\{U^t \mid t \geq 0\}$ if and only if L^* is the infinitesimal generator of the contraction semigroup $\{V^t \mid t \geq 0\}$ where $V^t \equiv (U^t)^*$.*

Using this theorem, the adjoint map produces a one-to-one inclusion reversing correspondence between the infinitesimal gen-

erators, of contraction semigroups, which are extensions of L and those which are restrictions of L^* . We label each of the latter with the $B \in \mathfrak{B}_1(M^\perp, \bar{N})$ of its adjoint, and call the infinitesimal generator, and its associated Cayley transform and semigroup, *extreme* if its adjoint is extreme by the previous definition. Since the adjoint map is continuous on $\mathfrak{B}_1(\mathcal{H})$, and the integral in (6) can be approximated by Riemann sums for the continuous integrand $U_{B'}^t$, Theorem 1 immediately implies

THEOREM 2. *If L is a densely defined dissipative operator on \mathcal{H} , every contraction semigroup $\{U_{B'}^t \mid t \geq 0\}$ which is generated by a restriction L_B of L^* can be represented in the form*

$$U_B^t = \int U_{B'}^t d\mu_B(B'), \quad t \geq 0 \quad (7)$$

where μ_B is a regular Borel probability measure concentrated on the extreme semigroups (and independent of t).

Now assume that $L = iH$ where H is symmetric and densely defined (which implies that L is dissipative). If for some conjugation K (i.e., antilinear isometric operator K on \mathcal{H} such that $K^2 = I$) we have

$$KHK = H \quad (8)$$

(i.e., H "permutes" with K) then it is natural to look for infinitesimal generators \tilde{L} satisfying either (a) $\tilde{L} \supseteq L$, or (b) $L \subseteq \tilde{L}^*$, and also

$$KLK = L^*. \quad (9)$$

In terms of Cayley transforms, (9) is equivalent to

$$KJK = J^* \quad (10)$$

and in terms of semigroups, (10) is equivalent to

$$KU^tK = (U^t)^*, \quad t \geq 0. \quad (11)$$

From (10) it follows that K is an (antilinear) isometry of $\text{Ran}(J)$ onto $\text{Ran}(J^*)$. Since H is symmetric, J is an isometry of $M = J^*J\mathcal{H} = \text{Ran}(J^*)$ onto $JJ^*\mathcal{H} = \text{Ran}(J)$, and from (8), K maps $\text{Ran}(J)$ isometrically onto $\text{Ran}(J^*)$. Therefore using the terminology of the proofs of Lemmas 1 and 2, \tilde{J} is of the form $\tilde{J} = J + B$ and $B(z) = UR(z) + zV = U + zV$. From the above remarks, K maps F isometrically onto G and $F^\perp = M^\perp \ominus F$ isometrically onto

$G^\perp = \bar{N} \ominus G$. Therefore V can be chosen to be an isometry of F^\perp onto G^\perp and for this choice $B[\exp(i\theta)]$, and $U_{B[\exp(i\theta)]}^t$, will be unitary. It is easy to choose V so as to also satisfy $KVK = V^*$, so that $KU_{B[\exp(i\theta)]}^tK = (U_{B[\exp(i\theta)]}^t)^*$.

DEFINITION. A contraction semigroup which satisfies (11) will be said to be *reflective* (with respect to the conjugation K).

We summarize the above argument in a corollary:

COROLLARY 1 (resp. 2) to Theorem 1 (resp. 2). *If furthermore $L = iH$, where H is symmetric and permutes with a conjugation K , then if U_{B^t} is reflective, the representation (6) (resp. (7)) of U_{B^t} can be made in terms of reflective, unitary U_{B^t} .*

We note that Corollaries 1 and 2 apply quite generally to Schrödinger equations in bounded regions.

The proof of Corollaries 1 and 2 can be simplified for H any densely defined symmetric operator with equal and finite deficiency indices; in such a case $\mathcal{B}_E(M^\perp, \bar{N})$ consists only of isometries of M^\perp onto \bar{N} , so the extreme semigroups are unitary, and there is no need for a conjugation operator.

Finally, we wish to consider the connection between the above results, and that of Nelson in [2]. In [2], Nelson solves (1) for $\mathcal{H} = L_2(\mathbf{R}^n)$, and $L = i(-\nabla^2 + V)$, where V is the multiplication operator on \mathcal{H} corresponding to any real function $V(x)$ continuous off a closed set S of capacity zero. Since the allowed $V(x)$ may be highly singular on S , a traditional approach to solving (1) would require the selection of some boundary condition at S . But Nelson seems to avoid such considerations by analytically continuing the *unique* solution of an associated diffusion equation. As suggested by [5], where a specific example ($V(x) = -(|c|/|x|)^2, n = 3$) is thoroughly examined, it seems reasonable to suspect that Nelson's analytic continuation technique is in general merely a method of averaging over time reversible evolutions in the sense of (6) or (7). This indeed follows immediately from our Corollary 1 since the hypotheses are easily seen to be satisfied with K the complex conjugation operator on $L_2(\mathbf{R}^n)$. It is suggestive that the averaging schemes (6) and (7) are superimposed in [2] on the stochastic aspects of Feynman and Wiener integrals for domains with boundary.

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