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An integral formula for section determinants of semi-groups of linear operators*

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Abstract. We derive an integral formula that expresses the section determinants of semi-groups of linear operators through the solution to a linear integral equation. The solution theory of this integral equation is developed and for a special case a concrete solvability criterion is presented.

1. Introduction

In quantum mechanics computing transition probabilities in many-fermion systems leads to section determinants of unitary operators, which are solutions to Schrödinger equations. Here we study, more generally, section determinants of semi-groups of linear operators, for which we derive an integral formula. To be more precise, let $U(t)$ be a semi-group of bounded, linear operators acting on a Hilbert space $\mathcal{H}$ and let $P : \mathcal{H} \to \mathcal{H}$ be an orthogonal projection having finite-dimensional range. We consider the determinant $\det(PU(T)P)$, which is to be understood as the determinant of the finite-dimensional operator $PU(T)P : \operatorname{ran} P \to \operatorname{ran} P$. In order to derive a formula for $\det(PU(T)P)$ we assume that the generator A of $U(t)$ has the form $A = A_0 + B$. In theorem 2.9 we prove the following formula:

$$\det(PU(T)P) = \det(PU_0(T)P) \exp\left[\int_0^1 \int_0^T \operatorname{tr}(B\,G(t, t+0; \alpha))\,\mathrm{d}t\,\mathrm{d}\alpha\right]. \tag{1}$$

Here $U_0(t)$ is the semi-group generated by A_0. The operator $G(t, t'; \alpha)$ solves the integral equation

$$G(t, t'; \alpha)\,\varphi = G_0(t, t')\,\varphi - \alpha \int_0^T G_0(t, \tau)\,B\,G(\tau, t'; \alpha)\,\varphi\,\mathrm{d}\tau \qquad \varphi \in \mathcal{H} \tag{2}$$

where the operator $G_0(t, t')$ can be expressed in terms of A_0 and P. $G(t, t'; \alpha)$ is called the time-ordered Green operator, although other names appear (see [1]). In the physics literature the solution to Schrödinger equations with time-dependent potentials is written as a formal exponential series, the so-called time-ordered exponential function. This may explain the name time-ordered Green operator.

A forerunner of formula (1) appears in Rivier and Simanek [5], who use a different version in order to compute the exact asymptotics in Anderson's orthogonality theorem. They do not

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give a rigorous proof but only indicate a formal derivation based upon manipulating infinite series within a Fock space formalism.

A special kind of equation (2) was formerly studied by Bart *et al* [1]. We shall not use their results here but develop independently a solution theory in section 3 that focuses completely on the special right-hand side $G_0(t, t')$, thus avoiding superfluous calculations. It will turn out that non-vanishing of the determinant $\det(PU(T, \alpha)P)$ and unique solvability of the integral equation are equivalent. In spite of being important as a theoretical tool this solvability criterion is unsuitable for practical purposes because, as we mentioned at the beginning, it is the determinant that will be the object of study. Thus it is important to have a solvability criterion that is formulated solely in terms of the generator A rather than the semi-group $U(t)$ itself. For the special case of $A = -\mathrm{i}H$, H being a self-adjoint operator, such a criterion will be presented in section 4. Since in that case $U(t)$ is a group of unitary operators our results may find applications in quantum mechanics.

Applications of formula (1) are not restricted to quantum mechanics, i.e. to the Schrödinger equation. Because we required that $U(t)$ be only a semi-group rather than a group we can use (1) to investigate section determinants related to other evolution equations such as, for instance, the heat equation. Therefore, our formula provides a new tool in the context of the so-called Szegö theorems.

In a comparably abstract framework section determinants of exponential-like operators were first investigated by Widom [6] who considered operators e^X, with X being trace class. His main tool was a factorization theorem based upon a general addition formula for operator-valued exponential functions known as Baker–Campbell–Hausdorff formula, which is important in the theory of Lie groups and Lie algebras.

2. The integral formula

Let $\mathcal{H}$ be a complex Hilbert space. We recall some basic facts concerning semi-groups. For details and proofs we refer to [3] and usually omit references at later points. A family of operators $U(t)$, $t \geqslant 0$, is called a strongly continuous semi-group of bounded linear operators, hereafter simply called the semi-group, if the following conditions are satisfied:

(a) for every $t \geqslant 0$, $U(t) : \mathcal{H} \to \mathcal{H}$ is a bounded linear operator,
(b) for every $\varphi \in \mathcal{H}$ the function $t \mapsto U(t)\,\varphi$, $t \geqslant 0$, is continuous,
(c) $U(0) = \mathbb{I}$,
(d) for every $t_1, t_2 \geqslant 0$, $U(t_1 + t_2) = U(t_1)\,U(t_2)$.

Here $\mathbb{I} : \mathcal{H} \to \mathcal{H}$ is the identity operator. Condition (b) is the strong continuity and condition (d) is the semi-group property. The norm of all $U(t)$ can be estimated by

$$\|U(t)\| \leqslant M\mathrm{e}^{\omega t} \qquad t \geqslant 0 \tag{3}$$

with constants $M \geqslant 1$ and $\omega \geqslant 0$.

The generator A of a semi-group is defined by

$$D(A) := \left\{\varphi \in \mathcal{H} \mid \lim_{t\to+0} \frac{1}{t}(U(t) - \mathbb{I})\,\varphi \text{ exists}\right\}$$

and

$$A : D(A) \to \mathcal{H} \qquad A\varphi := \lim_{t\to+0} \frac{1}{t}(U(t) - \mathbb{I})\,\varphi.$$

A semi-group possesses exactly one generator, which is a linear, densely defined, closed operator. Conversely, a linear operator can generate at most one semi-group. The semi-group

$U(t)$ leaves invariant $D(A)$, i.e. $U(t)\,\varphi \in D(A)$ for $\varphi \in D(A)$. Moreover, for $\varphi \in D(A)$ the function $t \mapsto U(t)\,\varphi$ is even differentiable rather than continuous and we have a differential equation:

$$\frac{\mathrm{d}}{\mathrm{dt}} U(t)\varphi = AU(t)\,\varphi \qquad t \geqslant 0 \tag{4}$$

for all $\varphi \in D(A)$. Conversely, the initial value problem

$$\frac{\mathrm{d}}{\mathrm{dt}} \varphi(t) = A\varphi(t) \qquad \varphi(0) \in D(A) \tag{5}$$

has exactly one solution, which is given by

$$\varphi(t) = U(t)\,\varphi(0). \tag{6}$$

Let $P : \mathcal{H} \to \mathcal{H}$ be an orthogonal projection having finite-dimensional range ran P. We are interested in the section determinant $\det(PU(T)P)$, which is meant as the determinant of the finite-dimensional operator $PU(T)P$: ran $P \to$ ran P. The source for our entire investigations is a well known formula that generalizes the logarithmic derivative of a scalar-valued function to the matrix case.

Lemma 2.1. *Let $\mathcal{K}$ be a finite-dimensional Hilbert space and $S(\alpha) : \mathcal{K} \to \mathcal{K}$, $\alpha_0 \leqslant \alpha \leqslant \alpha_1$, be a family of invertible linear operators depending continuously differentiably on α in the operator norm. Then the following formula holds:*

$$\frac{\mathrm{d}}{\mathrm{d}\alpha} \ln \det S(\alpha) = \operatorname{tr}(S^{-1}(\alpha) S'(\alpha)). \tag{7}$$

Here a prime denotes the derivative with respect to α and tr *is the trace.*

Proof. Let $s_1(\alpha), \dots, s_N(\alpha)$ denote the column vectors of $S(\alpha)$ where $N := \dim \mathcal{K}$. Then,

$$\frac{\mathrm{d}}{\mathrm{d}\alpha} \det S(\alpha) = \sum_{k=1}^{N} \det(s_1(\alpha), \dots, s_{k-1}(\alpha), s_k'(\alpha), s_{k+1}(\alpha), \dots, s_N(\alpha)).$$

Now expand the kth summand by the kth column and recall Cramer's rule to conclude that

$$\frac{\mathrm{d}}{\mathrm{d}\alpha} \det S(\alpha) = \det S(\alpha) \operatorname{tr}(S^{-1}(\alpha) S'(\alpha)).$$

This proves the lemma. □

The trace in lemma 2.1 is the reason why we need some simple facts about trace class operators in the course of this paper. We generally refer to [4] for the necessary prerequisites.

It is easily seen by using standard arguments that $\operatorname{tr}(S^{-1}(\alpha)S'(\alpha))$ depends continuously on α, whence we may integrate the above formula. Exponentiating yields

$$\det S(\alpha_1) = \det S(\alpha_0) \exp\left[\int_{\alpha_0}^{\alpha_1} \operatorname{tr} S^{-1}(\alpha) S'(\alpha)\, \mathrm{d}\alpha\right]. \tag{8}$$

In order to apply this formula to $\det(PU(T)P)$ we introduce a new parameter α instead of differentiating by T which would lead to a nonlinear differential equation, the so-called Riccati equation (see [2]). Let the generator A be decomposed into

$$A = A_0 + B. \tag{9}$$

We assume that $A_0 : D(A_0) \to \mathcal{H}$ generates a semi-group $U_0(t)$ and that $B : \mathcal{H} \to \mathcal{H}$ is bounded. Now define the operator pencil $A(\alpha)$ by

$$A(\alpha) := A_0 + \alpha B \qquad \alpha \in [0, 1]. \tag{10}$$

Since B is bounded $A(\alpha)$ is defined on $D(A_0)$. Moreover, since A_0 generates a semi-group so does $A(\alpha)$. We shall denote the semi-group generated by $A(\alpha)$ by $U(t,\alpha)$ throughout this paper. It is obvious that $U_0(t) = U(t,0)$ and $U(t) = U(t,1)$. We have the estimate:

$$\|U(t,\alpha)\| \leqslant M\mathrm{e}^{(\omega+\alpha M\|B\|)t} \qquad t \geqslant 0 \qquad \alpha \in [0,1] \tag{11}$$

where the constants $M \geqslant 1$ and $\omega \geqslant 0$ are independent of α.

In order to apply formula (8) to the finite-dimensional operator $PU(T,\alpha)P : \operatorname{ran} P \to \operatorname{ran} P$ we need to extend the inverse $(PU(T,\alpha)P)^{-1}$ to the whole of $\mathcal{H}$ and to compute the derivative $\partial U(T,\alpha)/\partial\alpha$. We start by introducing the so-called pseudo inverse relative to P.

Lemma 2.2. *Let $S : \mathcal{H} \to \mathcal{H}$ be a linear operator and $P : \mathcal{H} \to \mathcal{H}$ an orthogonal projection such that the operator $(PSP|_{\operatorname{ran} P})^{-1} : \operatorname{ran} P \to \operatorname{ran} P$ exists. We define the operator $S^+ : \mathcal{H} \to \mathcal{H}$ as follows. First we define*

$$S^+\varphi := \begin{cases} (PSP|_{\operatorname{ran} P})^{-1}\varphi & \text{for } \varphi \in \operatorname{ran} P \\ 0 & \text{for } \varphi \in (\operatorname{ran} P)^\perp \end{cases}$$

and then extend S^+ by linearity to the whole of $\mathcal{H}$. Then we have $S^+ = S^+P = PS^+$ and $S^+SP = PSS^+ = P$. If in addition S and P commute we have $SS^+ = S^+S = P$. We call S^+ pseudo inverse of S relative to P.

Proof. We have

$$S^+\varphi = S^+P\varphi + S^+(\mathbb{I} - P)\,\varphi = S^+P\varphi + 0.$$

Thus $S^+ = S^+P$. Since S^+: $\operatorname{ran} P \to \operatorname{ran} P$ it follows that $S^+P\varphi \in \operatorname{ran} P$ and hence $S^+P\varphi = PS^+P\varphi$. This gives $S^+ = PS^+$. Moreover, we have

$$S^+SP\varphi = S^+PSP\varphi + S^+(\mathbb{I} - P)SP\varphi = P\varphi + 0$$

and by the first part

$$PSS^+\varphi = PSPS^+\varphi = P\varphi.$$

If S and P commute it follows from what has been proved so far that

$$SS^+ = SPS^+ = PSS^+ = P$$

and analogously $S^+S = P$. This completes the proof. □

We turn to computing the derivative $\partial U(T,\alpha)/\partial\alpha$. We recall an integral equation that will also be useful below. In the following all integrals involving operators are meant as integrals in the strong sense.

Lemma 2.3. *Let $S_0 : D(S_0) \to \mathcal{H}$ be the generator of a semi-group $U_0(t)$ and $S_1 : \mathcal{H} \to \mathcal{H}$ be bounded. If $U(t)$ is the semi-group generated by $S_0 + S_1$ then for $0 \leqslant t_0 \leqslant t_1$ and all $\varphi \in \mathcal{H}$ we have*

$$(U(t_1) - U_0(t_1 - t_0)U(t_0))\,\varphi = \int_{t_0}^{t_1} U_0(t_1 - \tau)S_1U(\tau)\,\varphi\,\mathrm{d}\tau. \tag{12}$$

Proof. See [3], section 3.1. The function $\tau \mapsto U_0(t_1 - \tau)\,U(\tau)\,\varphi$ is differentiable for $\varphi \in D(S_0) = D(S_0 + S_1)$ and we have

$$\frac{\mathrm{d}}{\mathrm{d}\tau}(U_0(t_1 - \tau)\,U(\tau)\,\varphi) = U_0(t_1 - \tau)\,S_1\,U(\tau)\,\varphi.$$

Integrating from t_0 to t_1 yields (12) for $\varphi \in D(S_0)$. Since $U_0(t)$, $U(t)$, and S_1 are bounded the formula is valid for all $\varphi \in \mathcal{H}$. □

In later applications formula (12) will be multiplicated by bounded operators. Then we shall use the fact that multiplication by a bounded operator and integration can be interchanged. Lemma 2.3 enables us to compute the derivative $\partial U(t,\alpha)/\partial\alpha$.

Lemma 2.4. *For every fixed $t \geqslant 0$ the semi-group $U(t,\alpha)$ depends continuously differentiably on α in the operator norm. For all $\varphi \in \mathcal{H}$ we have*

$$\left(\frac{\partial}{\partial\alpha}U(t,\alpha)\right)\varphi = \int_0^t U(t-\tau,\alpha)\,B\,U(\tau,\alpha)\,\varphi\,\mathrm{d}\tau. \tag{13}$$

Proof. We consider the difference quotient. Put $S_0 := A_0 + \alpha B$ and $S_1 := hB$ and $t_0 := 0$, $t_1 := t$ in lemma 2.3:

$$U(t,\alpha+h)\,\varphi = U(t,\alpha)\,\varphi + h\int_0^t U(t-\tau,\alpha)\,B\,U(\tau,\alpha+h)\,\varphi\,\mathrm{d}\tau \qquad \varphi\in\mathcal{H}. \tag{14}$$

Iterating (14) and rearranging for the difference quotient yield:

$$\begin{aligned}\frac{1}{h}(U(t,\alpha+h)\,\varphi - U(t,\alpha)\,\varphi) &= \int_0^t U(t-\tau,\alpha)\,B\,U(\tau,\alpha)\,\varphi\,\mathrm{d}\tau \\ &\quad + h\int_0^t U(t-\tau,\alpha)\,B\int_0^\tau U(\tau-\tau',\alpha)\,B\,U(\tau',\alpha+h)\,\varphi\,\mathrm{d}\tau'\,\mathrm{d}\tau. \end{aligned} \tag{15}$$

Then (15) shows by using the estimate in (11) that the difference quotient converges in the operator norm and that formula (13) is correct. The continuity of $\partial U(t,\alpha)/\partial\alpha$ with respect to α follows in a similar way. □

Thus far, we have collected all the necessary prerequisites that enable us to formulate a preliminary version of the integral formula.

Proposition 2.5. *Let $T \geqslant 0$ be fixed and assume* $\det(PU(T,\alpha)P) \neq 0$ *for all* $\alpha \in [0,1]$. *Let $U^+(T,\alpha)$ be the pseudo inverse of $U(T,\alpha)$ relative to P according to lemma 2.2. Then we have*

$$\det(PU(T)P) = \det(PU_0(T)P)\exp\left[\int_0^1\int_0^T \operatorname{tr} B\,U(t,\alpha)\,U^+(T,\alpha)\,U(T-t,\alpha)\,\mathrm{d}t\,\mathrm{d}\alpha\right]. \tag{16}$$

Proof. By lemma 2.4 $U(T,\alpha)$ is continuously differentiable in the operator norm with respect to α. Together with $\det(PU(T,\alpha)P) \neq 0$ the finite-dimensional operator $PU(T,\alpha)P$: $\operatorname{ran} P \to \operatorname{ran} P$ satisfies the assumptions of lemma 2.1. Since $U(T,0) = U_0(T)$ and $U(T,1) = U(T)$ it follows:

$$\det(PU(T)P) = \det(PU_0(T)P)\exp\left[\int_0^1 \operatorname{tr}\left(U^+(T,\alpha)\frac{\partial U(T,\alpha)}{\partial\alpha}\right)\mathrm{d}\alpha\right].$$

Because of the appearance of $U^+(T,\alpha)$ the trace refers only to the finite-dimensional space $\operatorname{ran} P$. Therefore, we may insert formula (13):

$$\begin{aligned}\operatorname{tr}\left[U^+(T,\alpha)\frac{\partial U(T,\alpha)}{\partial\alpha}\right] &= \int_0^T \operatorname{tr}(U^+(T,\alpha)\,U(T-t,\alpha)\,B\,U(t,\alpha))\,\mathrm{d}t \\ &= \int_0^T \operatorname{tr}(B\,U(t,\alpha)\,U^+(T,\alpha)\,U(T-t,\alpha))\,\mathrm{d}t.\end{aligned}$$

Here we have used the cyclic commutativity under the trace. This proves the statement. □

In order to describe the expression $U(t,\alpha)\,U^+(T,\alpha)\,U(T-t,\alpha)$ independently of $U(t,\alpha)$ we introduce the Green operators.

Definition 2.6. *Let $T \geqslant 0$ be fixed and assume* $\det(PU(T,\alpha)P) \neq 0$. *Let $U^{+}(T,\alpha)$ be the pseudo inverse of $U(T,\alpha)$ relative to P. The operator defined by ($0 \leqslant t, t' \leqslant T$)*

$$G(t,t';\alpha) := \begin{cases} U(t,\alpha)\,U^{+}(T,\alpha)\,U(T-t',\alpha) & t \leqslant t' \\ U(t,\alpha)\,U^{+}(T,\alpha)\,U(T-t',\alpha) - U(t-t',\alpha) & t > t' \end{cases}$$

is called the time-ordered Green operator. The special case $\alpha = 0$ is abbreviated to $G_0(t,t') := G(t,t';0)$ *and called the free time-ordered Green operator.*

Of course, $G(t,t';\alpha)$ depends on T. We do not indicate this because otherwise we have too many variables. Sometimes $G(t,t';\alpha)$ is called the bi-semi-group generated by A (see [1]), but we prefer the name time-ordered Green operator, which is motivated by physical applications. The name Green operator will be justified in section 3. We note the properties of $G(t,t';\alpha)$.

Lemma 2.7. *Let $G(t,t';\alpha)$ be the time-ordered Green operator according to definition 2.6. Then the function $t \mapsto G(t,t';\alpha)$ is strongly continuous for $0 \leqslant t \leqslant T$, $t \neq t'$, and all $0 \leqslant t' \leqslant T$. For* $0 \leqslant t \leqslant t' \leqslant T$ *and all* $\alpha \in [0,1]$ *the operators $G(t,t';\alpha)$ and $B\,G(t,t';\alpha)$ are trace class. Moreover, the limit*

$$\operatorname{tr} B\,G(t,t+0;\alpha) := \lim_{\substack{t'\to t\\ t'\geqslant t}} \operatorname{tr} B\,G(t,t';\alpha)$$

exists and the function $\operatorname{tr} B\,G(t,t+0;\alpha)$ *depends continuously on t and α.*

Proof. The strong continuity of $G(\cdot,t';\alpha)$ (for $t \neq t'$) follows immediately from the strong continuity of $U(t,\alpha)$ and the definition of $G(t,t';\alpha)$.

Since $U^{+}(T,\alpha) = PU^{+}(T,\alpha)$ has a finite-dimensional range and thus is trace class, $G(t,t+0;\alpha)$ and $B\,G(t,t+0;\alpha)$ are trace class too. The existence and continuity of $\operatorname{tr} B\,G(t,t+0;\alpha)$ follows for the same reason. □

Now we are prepared to derive an integral equation that connects $G(t,t';\alpha)$ to $G_0(t,t')$.

Proposition 2.8. *The time-ordered Green operator according to definition 2.6 satisfies the integral equation*

$$G(t,t';\alpha)\,\varphi = G_0(t,t')\,\varphi - \alpha \int_0^T G_0(t,\tau)\,B\,G(\tau,t';\alpha)\,\varphi\,\mathrm{d}\tau \tag{17}$$

with $\varphi \in \mathcal{H}$, $0 \leqslant t, t' \leqslant T$ *and* $\alpha \in [0,1]$.

Proof. Let $t \leqslant t'$. Splitting up the integral in (17) and inserting the definitions of G_0 and G yields

$$\begin{aligned} I &:= \alpha \int_0^T G_0(t,\tau)\,B\,G(\tau,t';\alpha)\,\varphi\,\mathrm{d}\tau \\ &= \alpha \int_0^T U_0(t)\,U_0^{+}(T)\,U_0(T-\tau)B\,U(\tau,\alpha)\,U^{+}(T,\alpha)\,U(T-t',\alpha)\,\varphi\,\mathrm{d}\tau \\ &\quad - \alpha \int_0^t U_0(t-\tau)\,B\,U(\tau,\alpha)\,U^{+}(T,\alpha)\,U(T-t',\alpha)\,\varphi\,\mathrm{d}\tau \\ &\quad - \alpha \int_{t'}^T U_0(t)\,U_0^{+}(T)\,U_0(T-\tau)\,B\,U(\tau-t',\alpha)\,\varphi\,\mathrm{d}\tau. \end{aligned}$$

After having substituted $\tau' = \tau - t'$ in the third integral we apply lemma 2.3:

$$\begin{aligned} I = {} & U_0(t)\, U_0^+(T)(U(T,\alpha) - U_0(T))\, U^+(T,\alpha)\, U(T-t',\alpha)\,\varphi \\ & -(U(t,\alpha) - U_0(t))U^+(T,\alpha)\, U(T-t',\alpha)\,\varphi \\ & -U_0(t)\, U_0^+(T)(U(T-t',\alpha) - U_0(T-t'))\,\varphi. \end{aligned}$$

This can be simplified with the aid of lemma 2.2, which tells us $U_0^+(T)\, U(T,\alpha)\, U^+(T,\alpha) = U_0^+(T)$ and $U_0^+(T)\, U_0(T)\, U^+(T,\alpha) = U^+(T,\alpha)$. Hence,

$$\begin{aligned} I &= -U(t,\alpha)\, U^+(T,\alpha)\, U(T-t',\alpha)\,\varphi + U_0(t)\, U_0^+(T)\, U_0(T-t')\,\varphi \\ &= -G(t,t';\alpha)\,\varphi + G_0(t,t')\,\varphi. \end{aligned}$$

For $t > t'$ we start with the decomposition

$$\int_0^T = \int_0^{t'} + \int_{t'}^{t} + \int_t^T .$$

Then the proof can be completed by analogous calculations. □

The main theorem of this paper now follows by simply summarizing what has been proved up to now.

Theorem 2.9. *Let $U(t)$ be a semi-group with generator A being decomposed according to (9). Let the operator pencil $A(\alpha)$ be defined as*

$$A(\alpha) := A_0 + \alpha B \qquad \alpha \in [0,1]. \tag{18}$$

Then $A(\alpha)$ generates a semi-group $U(t,\alpha)$. Let $T \geqslant 0$ be fixed and assume $\det(PU(T,\alpha)P) \neq 0$ *for all $\alpha \in [0,1]$. Finally, denote by $G_0(t,t')$ the free time-ordered Green operator according to definition 2.6. Then the integral equation*

$$G(t,t';\alpha)\,\varphi = G_0(t,t')\,\varphi - \alpha \int_0^T G_0(t,\tau)\, B\, G(\tau,t';\alpha)\,\varphi\, \mathrm{d}\tau \tag{19}$$

with $\varphi \in \mathcal{H}$, $0 \leqslant t,t' \leqslant T$ and $\alpha \in [0,1]$ possesses at least one solution $G(t,t';\alpha)$, the time-ordered Green operator, having the properties:

(a) The function $t \mapsto G(t,t';\alpha)$ is strongly continuous for $0 \leqslant t \neq t'$ and all $0 \leqslant t'$ and all $\alpha \in [0,1]$.

(b) For $t \leqslant t'$ the operators $G(t,t';\alpha)$ and $B\, G(t,t';\alpha)$ are trace class and the function

$$\mathrm{tr}\, B\, G(t,t+0;\alpha) := \lim_{\substack{t'\to t\\ t'\geqslant t}} \mathrm{tr}\, B\, G(t,t';\alpha) \tag{20}$$

is well defined and continuously with respect to both t and α.

(c) For the section determinants there holds the integral formula

$$\det(PU(T)P) = \det(PU_0(T)P)\exp\left[\int_0^1 \int_0^T \mathrm{tr}\, B\, G(t,t+0;\alpha)\, \mathrm{d}t\, \mathrm{d}\alpha\right]. \tag{21}$$

Proof. Combine propositions 2.5 and 2.8. □

The statement of this theorem has a perturbation-like character in that it relates the determinant of the unperturbed operator A_0 to the determinant of the perturbed operator A. There is, of course, some freedom in choosing the decomposition $A = A_0 + B$. It seems to be reasonable to assume that P and A_0 commute. Then ran P is an invariant subspace for A_0 and we may consider the determinant associated with A_0 to be known. One extreme possibility is to take $A_0 = 0$ leading to a very simple G_0. In the other direction we may take the largest possible commuting operator to be A_0, that is $A_0 := PAP + (\mathbb{I} - P)A(\mathbb{I} - P)$; which is best will depend on the special situation.

3. Solution theory of the integral equation

The foregoing section suggests that the determinant $\det(PU(T,\alpha)P)$ is intimately related to the solution theory of the integral equation (19). In the following we shall analyse this relationship in detail. We shall show that uniqueness of the solution already implies existence of a solution for the special right-hand side in (19). Hence we only need to consider the homogeneous integral equation. First of all we show that the homogeneous equation is connected with a homogeneous boundary value problem. In this section the parameter α is not crucial. We retain it to stay in concordance with the notation of section 2.

The time-ordered Green operator $G(t,t';\alpha)$ satisfies, at least formally, a differential equation

$$\frac{\partial}{\partial t}G(t,t';\alpha) = -\delta(t-t')\mathbb{I} + A(\alpha)G(t,t';\alpha). \tag{22}$$

Here δ is the Dirac delta. Furthermore, we have simple boundary conditions.

Lemma 3.1. *The time-ordered Green operator $G(t,t';\alpha)$ according to definition 2.6 satisfies for all $\alpha \in [0,1]$ the boundary conditions*

$$(\mathbb{I}-P)G(0,t';\alpha) = 0 \qquad PG(T,t';\alpha) = 0 \qquad 0 \leqslant t' \leqslant T. \tag{23}$$

Proof. We note that $U^+(T,\alpha) = PU^+(T,\alpha)$ (see lemma 2.2):

$$\begin{aligned}(\mathbb{I}-P)G(0,t';\alpha) &= (\mathbb{I}-P)U(0,\alpha)\,U^+(T,\alpha)\,U(T-t',\alpha)\\ &= (\mathbb{I}-P)\,U^+(T,\alpha)\,U(T-t',\alpha)\\ &= 0.\end{aligned}$$

For $t = T$ we use $PU(T,\alpha)\,U^+(T,\alpha) = P$ (see lemma 2.2):

$$\begin{aligned}PG(T,t';\alpha) &= PU(T,\alpha)\,U^+(T,\alpha)\,U(T-t',\alpha) - PU(T-t',\alpha)\\ &= PU(T-t',\alpha) - PU(T-t',\alpha)\\ &= 0.\end{aligned}$$

This proves the lemma. □

Equation (22) and lemma 3.1 justify the name Green operator and motivate the following theorem.

Theorem 3.2. *Let the function $\varphi(\cdot) : t \mapsto \varphi(t) \in \mathcal{H}$ be continuously differentiable and solve the integral equation*

$$\varphi(t) = -\alpha\int_0^T G_0(t,\tau)\,B\varphi(\tau)\,\mathrm{d}\tau \qquad 0 \leqslant t \leqslant T. \tag{24}$$

Then $\varphi(\cdot)$ is also a solution to the boundary value problem:

$$\frac{\mathrm{d}}{\mathrm{dt}}\varphi(t) = A(\alpha)\,\varphi(t) \qquad (\mathbb{I}-P)\,\varphi(0) = 0 \qquad P\varphi(T) = 0. \tag{25}$$

Proof. We split up the integral in (24):

$$\begin{aligned}I(t) &:= \int_0^T G_0(t,\tau)\,B\varphi(\tau)\,\mathrm{d}\tau\\ &= \int_0^t (U_0(t)\,U_0^+(T)\,U_0(T-\tau) - U_0(t-\tau))\,B\varphi(\tau)\,\mathrm{d}\tau\\ &\quad + \int_t^T U_0(t)\,U_0^+(T)\,U_0(T-\tau)\,B\varphi(\tau)\,\mathrm{d}\tau.\end{aligned}$$

We have assumed that $\varphi(\,\cdot\,)$ is continuously differentiable. Then it is known from semi-group theory that the respective integrands are also continuously differentiable since all operators involved are bounded. Moreover, $I(\,\cdot\,)$ is continuously differentiable and $\varphi(\,\cdot\,)$ solves the differential equation (25). The boundary conditions are clear from lemma 3.1. □

The assumption that the solution to the integral equation is continuously differentiable generally does not follow from the integral equation when the generator A_0 is unbounded (see [3], section 4.2.) and therefore cannot be dropped. Theorem 3.2 has a converse.

Theorem 3.3. *Let the function $\varphi(\,\cdot\,) : t \mapsto \varphi(t) \in \mathcal{H}$ be continuously differentiable and let $\varphi(0) \in D(A)$. Then if $\varphi(\,\cdot\,)$ solves the boundary value problem (25) $\varphi(\,\cdot\,)$ is also a solution to the integral equation (24).*

Proof. Let $\varphi(\,\cdot\,)$ be a solution to (25). A look at (5) and (6) shows that $\varphi(t)$ can be written as

$$\varphi(t) = U(t,\alpha)\,\varphi(0)$$

since $\varphi(0) \in D(A)$. We evaluate the integral

$$I(t) := \alpha \int_0^T G_0(t,\tau)\, B\, U(\tau,\alpha)\,\varphi(0)\,\mathrm{d}\tau$$

with the aid of lemma 2.3 (see the proof of proposition 2.8 for related calculations). We split up the integral and insert the definition of $G_0(t,t')$:

$$\begin{aligned} I(t) &= \alpha \int_0^T U_0(t)\, U_0^+(T)\, U_0(T-\tau)\, B\, U(\tau,\alpha)\,\varphi(0)\,\mathrm{d}\tau - \alpha \int_0^t U_0(t-\tau)\, B\, U(\tau,\alpha)\,\varphi(0)\,\mathrm{d}\tau \\ &= U_0(t)\, U_0^+(T)(U(T) - U_0(T))\,\varphi(0) - (U(t) - U_0(t))\,\varphi(0). \end{aligned}$$

Now use the boundary conditions and recall the properties of the pseudo inverse from lemma 2.2 to conclude

$$I(t) = -U(t)\,\varphi(0) = -\varphi(t).$$

This proves the lemma. □

The solvability of the boundary value problem can be characterized by $\det(PU(T,\alpha)P)$.

Theorem 3.4. *The boundary value problem (25) only has the trivial solution if and only if* $\det(PU(T,\alpha)P) \neq 0$.

Proof. According to (5) and (6) the solution to the boundary value problem can be written as:

$$\varphi(t) = U(t,\alpha)\,\varphi(0).$$

From the boundary conditions it follows that $\varphi(0) = P\varphi(0)$ and

$$0 = P\varphi(T) = PU(T,\alpha)\,\varphi(0) = PU(T,\alpha)P\varphi(0).$$

Considering this equation on ran P shows that $\det(PU(T,\alpha)P) \neq 0$ is equivalent to $\varphi(0) = 0$. This proves the theorem. □

From the preceding considerations we obtain a criterion for the non-vanishing of the determinant $\det(PU(T,\alpha)P)$.

Corollary 3.5. *Let the homogeneous equation (24) only have the trivial solution. Then,*

(a) $\det(PU(T,\alpha)P) \neq 0$.
(b) The inhomogeneous integral equation (19) has exactly one solution.

Proof.

(a) If $\det(PU(T,\alpha)P) = 0$ the boundary value problem (25) has a non-trivial solution, which is also a non-trivial solution to the integral equation (24). This contradicts the assumption.

(b) Since the homogeneous equation (24) only has the trivial solution the inhomogeneous equation (19) can have at most one solution. Since $\det(PU(T,\alpha)P) \neq 0$ by (a), in definition 2.6 the operator $U^+(T,\alpha)$ exists. Thus by theorem 2.9 $G(t,t';\alpha)$ provides a solution to equation (19). □

The above solvability criterion reminds us of the Riesz theory for compact operators in that uniqueness of the solution implies existence of a solution. However, we have to note that the existence criterion only refers to the special right-hand side in (19).

4. A solvability criterion

In the preceding section we showed that the integral equation (24) and the boundary value problem (25) are equivalent. However, we have not yet given a practical criterion which ensures that either of the above problems only has the trivial solution. This will be done now for the boundary value problem in the special case $A = -\mathrm{i}H$ with $H : \mathcal{H} \to \mathcal{H}$ being a bounded, self-adjoint operator. The boundedness of H is not really essential but it helps to keep the presentation as simple as possible. The parameter α does not appear for the same reason. It is known (see [3]) that $-\mathrm{i}H$ generates a semi-group $U(t)$. Actually, $U(t)$ is even a group, i.e. t is allowed to take negative values. Each $U(t)$ is a unitary operator.

It will turn out to be convenient to write $\mathcal{H}$ as orthogonal sum $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$ with $\mathcal{H}_1 := \operatorname{ran} P$ and $\mathcal{H}_2 := \mathcal{H}_1^{\perp}$. Then, H can be represented as a block matrix:

$$H = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \qquad H_{jk} : \mathcal{H}_k \to \mathcal{H}_j \qquad j,k = 1,2. \tag{26}$$

Note, that the self-adjointness of H implies $H_{jk} = H_{kj}^*$, $j,k = 1,2$. If we had $H_{12} = 0$ and $H_{21} = 0$ then $\operatorname{ran} P$ would be an invariant subspace for H and the boundary value problem (25) would easily be seen to have only the trivial solution. In general this will not be the case. However, instead of being furnished with an invariant subspace it suffices that the operators H_{11} and H_{22} are separated from each other in some sense.

Theorem 4.1. *Let $H : \mathcal{H} \to \mathcal{H}$ be a bounded, self-adjoint operator. Assume*

$$H_{11} \leqslant \gamma\mathbb{I} < \Gamma\mathbb{I} \leqslant H_{22} \tag{27}$$

$\gamma, \Gamma \in \mathbb{R}$, in the sense of quadratic forms. Then the boundary value problem (25) with $A = -\mathrm{i}H$ possesses only the trivial solution $\varphi(t) = 0$.

Proof. Let $\varphi(t)$ be a solution to the boundary value problem (25). We write $\varphi = (\varphi_1, \varphi_2)^T$ according to $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$. The boundary conditions read

$$\varphi_2(0) = 0 \qquad \varphi_1(T) = 0. \tag{28}$$

Let $j \in \mathbb{N}_0$. By noting the self-adjointness of H we see

$$\frac{\mathrm{d}}{\mathrm{d}t}(\varphi(t), H^j\varphi(t)) = 2\,\mathrm{Re}(\varphi(t), H^j\varphi'(t)) = -2\,\mathrm{Re}\,\mathrm{i}(\varphi(t), H^{j+1}\varphi(t)) = 0.$$

Thus, $(\varphi(T), H^j\varphi(T)) = (\varphi(0), H^j\varphi(0))$. Put $j = 0, 1$ and use the boundary conditions (28) to obtain

$$\|\varphi_1(0)\|^2 = \|\varphi_2(T)\|^2 \tag{29}$$

$$(\varphi_1(0), H_{11}\varphi_1(0)) = (\varphi_2(T), H_{22}\varphi_2(T)). \tag{30}$$

In the last equality we can estimate via (27):

$$\gamma \|\varphi_1(0)\|^2 \geqslant \Gamma \|\varphi_2(T)\|^2.$$

Because of (29) and $\gamma < \Gamma$ this is only possible with $\|\varphi_1(0)\| = 0$ what implies $\varphi(t) = 0$ by (6). □

It is easy to see that (27) in the above theorem can be replaced by $H_{11} \geqslant \gamma \mathbb{I} > \Gamma \mathbb{I} \geqslant H_{22}$ without further ado.

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