

## THE LIFSHITZ–KREIN TRACE FORMULA AND OPERATOR LIPSCHITZ FUNCTIONS

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ABSTRACT. We solve a problem by M.G. Krein and describe the maximal class of functions  $f$  on the real line, for which the Lifshitz–Krein trace formula  $\text{trace}(f(A) - f(B)) = \int_{\mathbb{R}} f'(s)\xi(s) ds$  holds for arbitrary self-adjoint operators  $A$  and  $B$  with  $A - B$  in the trace class  $\mathcal{S}_1$ . We prove that this class of functions coincide with the class of operator Lipschitz functions.

### 1. INTRODUCTION

The purpose of this paper is to describe the class of functions, for which the Lifshitz–Krein trace formula holds. The Lifshitz–Krein trace formula plays a significant role in perturbation theory. It was discovered by Lifshitz [L] in a special case and by Krein [Kr] in the general case. This formula allows one to compute the trace of the difference  $f(A) - f(B)$  of a function  $f$  of an unperturbed self-adjoint operator  $A$  and a perturbed self-adjoint operator  $B$  provided the perturbation  $B - A$  belongs to trace class  $\mathcal{S}_1$ . M. G. Krein proved that for each such pair there exists a unique function  $\xi$  in  $L^1(\mathbb{R})$  such that for every function  $f$  whose derivative is the Fourier transform of a complex measure, the operator  $f(A) - f(B)$  belongs to  $\mathcal{S}_1$  and the following trace formula holds:

$$(1.1) \quad \text{trace}(f(A) - f(B)) = \int_{\mathbb{R}} f'(s)\xi(s) ds$$

(see [Kr]). The function  $\xi$  is called the *spectral shift function associated with the pair*  $(A, B)$ . Krein posed in [Kr] the problem to describe the maximal class of functions, for which trace formula (1.1) holds for arbitrary self-adjoint operators  $A$  and  $B$  with trace class difference.

Clearly, the right-hand side of (1.1) makes sense for arbitrary Lipschitz functions  $f$ . In this connection Krein asked the question of whether it is true that for an arbitrary Lipschitz function  $f$ , the operator  $f(A) - f(B)$  is in  $\mathcal{S}_1$  and trace formula (1.1) holds. *It turns out that this is false.* In [F] Farforovskaja gave an example of self-adjoint operators  $A$  and  $B$  with  $A - B \in \mathcal{S}_1$  and a Lipschitz function  $f$  such that  $f(A) - f(B) \notin \mathcal{S}_1$ .

Later it was shown in [Pe2] and [Pe3] that formula (1.1) holds, whenever  $A$  and  $B$  are self-adjoint operators with  $A - B \in \mathcal{S}_1$  and  $f$  belongs to the Besov

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space  $B_{\infty,1}^1(\mathbb{R})$  (we refer the reader to [Pee] and [Pe4] for an introduction to Besov classes). Necessary conditions are also obtained in [Pe2] and [Pe3]. In particular, it was shown in [Pe2] and [Pe3] that if  $f(A) - f(B) \in \mathbf{S}_1$  whenever  $A$  and  $B$  are self-adjoint operators with  $A - B \in \mathbf{S}_1$ , then  $f$  locally belongs to the Besov space  $B_{1,1}^1(\mathbb{R})$ . Note that those necessary conditions were deduced from the description of trace class Hankel operators [Pe1] (see also [Pe4]).

The main objective of this paper is to describe the class of functions  $f$ , for which trace formula (1.1) holds for arbitrary self-adjoint operators  $A$  and  $B$  with  $A - B \in \mathbf{S}_1$ .

It is well known (see e.g. [AP2]) that for a function  $f$  on  $\mathbb{R}$ , the following properties are equivalent:

(i) *there exists a positive number  $C$  such that*

$$(1.2) \quad \|f(A) - f(B)\| \leq C\|A - B\|$$

*for all bounded self-adjoint operators  $A$  and  $B$ ;*

(ii) *there exists a positive number  $C$  such that inequality (1.2) holds, whenever  $A$  and  $B$  are (not necessarily bounded) self-adjoint operators such that  $A - B$  is bounded;*

(iii) *there exists a positive number  $C$  such that*

$$(1.3) \quad \|f(A) - f(B)\|_{\mathbf{S}_1} \leq C\|A - B\|_{\mathbf{S}_1}$$

*for all bounded self-adjoint operators  $A$  and  $B$  with  $A - B \in \mathbf{S}_1$ ;*

(iv) *there exists a positive number  $C$  such that inequality (1.3) holds, whenever  $A$  and  $B$  are (not necessarily bounded) self-adjoint operators such that  $A - B \in \mathbf{S}_1$ ;*

(v)  *$f(A) - f(B) \in \mathbf{S}_1$ , whenever  $A$  and  $B$  are (not necessarily bounded) self-adjoint operators such that  $A - B \in \mathbf{S}_1$ .*

Note that the minimal value of the constant  $C$  is the same in (i)–(iv).

Functions satisfying (i) are called *operator Lipschitz*. We denote by  $\text{OL}(\mathbb{R})$  the space of operator Lipschitz functions on  $\mathbb{R}$ . For  $f \in \text{OL}(\mathbb{R})$ , we define its seminorm  $\|f\|_{\text{OL}}$  as the infimum of all constants  $C$ , for which inequality (1.2) holds. In other words,

$$\begin{aligned} \|f\|_{\text{OL}} &= \sup \left\{ \frac{\|f(A) - f(B)\|}{\|A - B\|} : A \text{ and } B \text{ are self-adjoint, } A - B \text{ is bounded} \right\} \\ &= \sup \left\{ \frac{\|f(A) - f(B)\|_{\mathbf{S}_1}}{\|A - B\|_{\mathbf{S}_1}} : A \text{ and } B \text{ are self-adjoint, } A - B \in \mathbf{S}_1 \right\}. \end{aligned}$$

It was shown in [JW] that operator Lipschitz functions are differentiable everywhere on  $\mathbb{R}$ . Note that this implies that the function  $x \mapsto |x|$  is not operator Lipschitz, the fact established earlier in [Mc] and [Ka]. On the other hand, an operator Lipschitz function does not have to be continuously differentiable; in particular, the function  $x \mapsto x^2 \sin x^{-1}$  is operator Lipschitz; see [KS].

For a differentiable function  $f$  on  $\mathbb{R}$ , we consider the divided difference  $\mathfrak{D}f$  defined by

$$(1.4) \quad (\mathfrak{D}f)(x, y) = \begin{cases} \frac{f(x) - f(y)}{x - y}, & x \neq y, \\ f'(x), & x = y. \end{cases}$$

It turns out (see e.g. [AP2]) that a differentiable function on  $\mathbb{R}$  is operator Lipschitz if and only if the divided difference  $\mathfrak{D}f$  is a Schur multiplier (see §2 for the definition).

The main purpose of this paper is to prove that *the condition  $f \in \text{OL}(\mathbb{R})$  is not only a necessary condition for the Lifshits–Krein trace formula (1.1) to hold for arbitrary self-adjoint operators  $A$  and  $B$  with  $A - B \in \mathcal{S}_1$ , but is also sufficient.* This will be proved in §6.

In §2 we define double operator integrals and Schur multipliers. In §3 we state a result of [KPSS] on the differentiability of the function  $t \mapsto f(A + tK) - f(A)$  in the Hilbert–Schmidt norm. We state a characterization of the space of Schur multipliers in terms of Haagerup tensor products in §4. Finally, in §5 we obtain a formula for the trace of double operator integrals.

## 2. DOUBLE OPERATOR INTEGRALS AND SCHUR MULTIPLIERS

Double operator integrals appeared in the paper [DK] by Daletskii and S. G. Krein. Later the beautiful theory of double operator integrals was created by Birman and Solomjak in [BS1], [BS2], and [BS4].

Let  $(\mathcal{X}, E_1)$  and  $(\mathcal{Y}, E_2)$  be spaces with spectral measures  $E_1$  and  $E_2$  on a Hilbert space  $\mathcal{H}$  and let  $\Phi$  be a bounded measurable function on  $\mathcal{X} \times \mathcal{Y}$ . Double operator integrals are expressions of the form

$$(2.1) \quad \int_{\mathcal{X}} \int_{\mathcal{Y}} \Phi(x, y) dE_1(x) T dE_2(y).$$

Birman and Solomjak’s starting point is the case when  $T$  belongs to the Hilbert–Schmidt class  $\mathcal{S}_2$ . For a bounded measurable function  $\Phi$  on  $\mathcal{X} \times \mathcal{Y}$  and an operator  $T$  of class  $\mathcal{S}_2$ , consider the spectral measure  $\mathcal{E}$  whose values are orthogonal projections on the Hilbert space  $\mathcal{S}_2$ , which is defined by

$$\mathcal{E}(\Lambda \times \Delta) T = E_1(\Lambda) T E_2(\Delta), \quad T \in \mathcal{S}_2,$$

$\Lambda$  and  $\Delta$  being measurable subsets of  $\mathcal{X}$  and  $\mathcal{Y}$ . It was shown in [BS5] that  $\mathcal{E}$  extends to a spectral measure on  $\mathcal{X} \times \mathcal{Y}$ . For a bounded measurable function  $\Phi$  on  $\mathcal{X} \times \mathcal{Y}$ , the double operator integral (2.1) is defined by

$$\int_{\mathcal{X}} \int_{\mathcal{Y}} \Phi(x, y) dE_1(x) T dE_2(y) \stackrel{\text{def}}{=} \left( \int_{\mathcal{X} \times \mathcal{Y}} \Phi d\mathcal{E} \right) T.$$

Clearly,

$$\left\| \int_{\mathcal{X}} \int_{\mathcal{Y}} \Phi(x, y) dE_1(x) T dE_2(y) \right\|_{\mathcal{S}_2} \leq \|\Phi\|_{L^\infty} \|T\|_{\mathcal{S}_2}.$$

If

$$\int_{\mathcal{X}} \int_{\mathcal{Y}} \Phi(x, y) dE_1(x) T dE_2(y) \in \mathcal{S}_1$$

for every  $T \in \mathcal{S}_1$ , we say that  $\Phi$  is a *Schur multiplier of  $\mathcal{S}_1$  associated with the spectral measures  $E_1$  and  $E_2$* . We denote by  $\mathfrak{M}(E_1, E_2)$  the space of Schur multipliers of  $\mathcal{S}_1$  with respect to  $E_1$  and  $E_2$ . The norm  $\|\Phi\|_{\mathfrak{M}(E_1, E_2)}$  of  $\Phi$  in the space

$\mathfrak{M}(E_1, E_2)$  is, by definition, the norm of the linear transformer

$$T \mapsto \int_{\mathcal{X}} \int_{\mathcal{Y}} \Phi(x, y) dE_1(x) T dE_2(y)$$

on the class  $\mathcal{S}_1$ .

If  $\Phi \in \mathfrak{M}(E_1, E_2)$ , one can define by duality double operator integrals of the form (2.1) for an arbitrary bounded linear operator  $T$ . However, we do not need this in this paper.

We are going to discuss briefly in § 4 characterizations of Schur multipliers.

Birman and Solomjak proved in [BS4] that if  $f$  is a Lipschitz function and  $A$  and  $B$  are not necessarily bounded self-adjoint operators with  $A - B \in \mathcal{S}_2$ , then

$$(2.2) \quad f(A) - f(B) = \iint_{\mathbb{R} \times \mathbb{R}} \frac{f(x) - f(y)}{x - y} dE_A(x)(A - B) dE_B(y).$$

Note that for an arbitrary Lipschitz function  $f$ , the divided difference  $\mathfrak{D}f$  is not always naturally defined on the diagonal. However, we can define  $\mathfrak{D}f$  on the diagonal by an arbitrary bounded measurable function and the right-hand side of (2.2) does not depend on the values on the diagonal. It follows from (2.2) that

$$\|f(A) - f(B)\|_{\mathcal{S}_2} \leq \|f\|_{\text{Lip}} \|A - B\|_{\mathcal{S}_2},$$

where the Lipschitz (semi)norm  $\|f\|_{\text{Lip}}$  of  $f$  is, by definition,

$$\sup \left\{ \frac{|f(x) - f(y)|}{|x - y|} : x, y \in \mathbb{R}, x \neq y \right\}.$$

On the other hand, if  $A$  and  $B$  are not necessarily bounded self-adjoint operators with  $A - B \in \mathcal{S}_1$  and  $f$  is an operator Lipschitz function, then

$$(2.3) \quad f(A) - f(B) = \iint_{\mathbb{R} \times \mathbb{R}} (\mathfrak{D}f)(x, y) dE_A(x)(A - B) dE_B(y);$$

(see [BS4]). Here the divided difference  $\mathfrak{D}f$  is defined by (1.4). It follows from (2.3) that

$$\|f(A) - f(B)\|_{\mathcal{S}_1} \leq \|f\|_{\text{OL}} \|A - B\|_{\mathcal{S}_1}.$$

### 3. DIFFERENTIABILITY IN THE HILBERT-SCHMIDT NORM

Suppose that  $A$  and  $B$  are not necessarily bounded self-adjoint operators on Hilbert space such that  $A - B \in \mathcal{S}_2$ . Consider the parametric family  $A_t, 0 \leq t \leq 1$ , defined by  $A_t = A + tK$ , where  $K \stackrel{\text{def}}{=} B - A$ . We need the following result of [KPSS], Theorem 7.18:

*Suppose that  $f$  is a Lipschitz function on  $\mathbb{R}$  that is differentiable at every point of  $\mathbb{R}$ . Then the function  $s \mapsto f(A_s) - f(A)$  is differentiable on  $[0, 1]$  in the Hilbert-Schmidt norm and*

$$\frac{d}{ds} (f(A_s) - f(A)) \Big|_{s=t} = \iint_{\mathbb{R} \times \mathbb{R}} (\mathfrak{D}f)(x, y) dE_t(x) K dE_t(y).$$

4. SCHUR MULTIPLIERS AND HAAGERUP TENSOR PRODUCTS

Let  $(\mathcal{X}, E_1)$  and  $(\mathcal{Y}, E_2)$  be spaces with spectral measures  $E_1$  and  $E_2$  on Hilbert space. There are several characterizations of the class  $\mathfrak{M}(E_1, E_2)$  of Schur multipliers; see [Pe2], [P1], [AP2]. We need the following characterization in terms of the Haagerup tensor product of  $L^\infty$  spaces:

*Let  $\Phi$  be a measurable function on  $\mathcal{X} \times \mathcal{Y}$ . Then  $\Phi \in \mathfrak{M}(E_1, E_2)$  if and only if  $\Phi$  belongs to the Haagerup tensor product  $L^\infty(E_1) \otimes_h L^\infty(E_2)$ , i.e.,  $\Phi$  admits a representation*

$$\Phi(x, y) = \sum_n \varphi_n(x)\psi_n(y),$$

where  $\varphi_n \in L^\infty(E_1)$ ,  $\psi_n \in L^\infty(E_2)$ , and

$$\sum_n |\varphi_n|^2 \in L^\infty(E_1) \quad \text{and} \quad \sum_n |\psi_n|^2 \in L^\infty(E_2).$$

Suppose now that  $E_1$  and  $E_2$  are Borel spectral measures on locally compact topological spaces  $\mathcal{X}$  and  $\mathcal{Y}$ . Suppose also that one of them is separable, and  $\text{supp } E_1 = \mathcal{X}$  and  $\text{supp } E_2 = \mathcal{Y}$ . In this case the following result holds (see [AP2]):

*Let  $\Phi$  be a function on  $\mathcal{X} \times \mathcal{Y}$  that is continuous in each variable. Then  $\Phi \in \mathfrak{M}(E_1, E_2)$  if and only if it belongs to the Haagerup tensor product  $C_b(\mathcal{X}) \otimes_h C_b(\mathcal{Y})$  of the spaces of bounded continuous functions on  $\mathcal{X}$  and  $\mathcal{Y}$ , i.e.,  $\Phi$  admits a representation*

$$\Phi(x, y) = \sum_n \varphi_n(x)\psi_n(y),$$

where  $\varphi_n \in C_b(\mathcal{X})$ ,  $\psi_n \in C_b(\mathcal{Y})$  and the functions

$$\sum_n |\varphi_n|^2 \quad \text{and} \quad \sum_n |\psi_n|^2$$

are bounded.

5. THE TRACE OF DOUBLE OPERATOR INTEGRALS

Let  $T$  be a trace class operator on a Hilbert space and let  $E$  be a spectral measure on a  $\sigma$ -algebra of subsets of a set  $\mathcal{X}$ . If  $\Phi$  is a Schur multiplier, i.e.,  $\Phi \in \mathfrak{M}(E, E)$ , then the double operator integral

$$\iint \Phi(x, y) dE(x)T dE(y)$$

belongs to  $\mathbf{S}_1$ . Let us compute its trace. In [BS4] the following trace formula was suggested:

$$(5.1) \quad \text{trace} \left( \iint \Phi(x, y) dE(x)T dE(y) \right) = \int \Phi(x, x) d\mu(x),$$

where  $\mu$  is the complex measure defined by

$$\mu(\Delta) = \text{trace} (TE(\Delta)).$$

The problem is how we can interpret the function  $x \mapsto \Phi(x, x)$  for functions  $\Phi$  in  $\mathfrak{M}(E, E)$ . In [Pe5] the following justification of formula (5.1) was given. We can

define the trace  $\mathcal{T}\Phi$  of a function  $\Phi$  in  $\mathfrak{M}(E, E)$  on the diagonal by the formula

$$(\mathcal{T}\Phi)(x) \stackrel{\text{def}}{=} \sum_n \varphi_n(x)\psi_n(x),$$

where

$$(5.2) \quad \Phi(x, y) = \sum_n \varphi_n(x)\psi_n(y)$$

is a representation of  $\Phi$  as an element of the Haagerup tensor product  $L^\infty(E) \otimes_h L^\infty(E)$ , i.e.,

$$(5.3) \quad \sum_m |\varphi_n|^2 \in L^\infty(E) \quad \text{and} \quad \sum_m |\psi_n|^2 \in L^\infty(E).$$

Clearly, the trace of  $\Phi \in \mathfrak{M}(E, E)$  on the diagonal belongs to  $L^\infty(E)$ . Then formula (5.1) holds if  $\Phi(x, x)$  is understood as  $(\mathcal{T}\Phi)(x)$ ; see [Pe5, § 1.1].

Suppose now that  $E$  is a Borel spectral measure on a locally compact topological space  $\mathcal{X}$  and  $\Phi$  is a function on  $\mathcal{X} \times \mathcal{X}$  that is continuous in each variable. Clearly, it suffices to consider the case when  $\text{supp } E = \mathcal{X}$ . As we have mentioned in § 2,  $\Phi$  admits a representation of the form (5.2), in which the functions  $\varphi_n$  and  $\psi_n$  satisfy (5.3) and are continuous functions on  $\mathcal{X}$ . It is easy to see that in this case  $(\mathcal{T}\Phi)(x) = \Phi(x, x)$ ,  $x \in \mathcal{X}$ . In other words, the following theorem holds:

**Theorem 5.1.** *Let  $E$  be a spectral measure on a locally compact topological space  $\mathcal{X}$ . Suppose that  $\Phi$  is a function of class  $\mathfrak{M}(E, E)$ . If  $\Phi$  is continuous in each variable, then formula (5.1) holds for an arbitrary trace class operator  $T$ .*

### 6. THE LIFSHITZ–KREIN TRACE FORMULA FOR ARBITRARY OPERATOR LIPSCHITZ FUNCTIONS

Suppose that  $A$  and  $B$  are self-adjoint operators on Hilbert space such that  $A - B \in \mathcal{S}_1$ . Let  $\xi$  be the spectral shift function associated with the pair  $(A, B)$ . As we have mentioned in § 2, for an arbitrary operator Lipschitz function  $f$  on  $\mathbb{R}$ , the operator  $f(A) - f(B)$  belongs to a trace class. The following theorem is the main result of the paper.

**Theorem 6.1.** *Let  $f \in \text{OL}(\mathbb{R})$ . Then*

$$\text{trace}(f(A) - f(B)) = \int_{\mathbb{R}} f'(s)\xi(s) ds.$$

To prove the theorem, we are going to use an approach of Birman and Solomjak in [BS3] to the Lifshitz–Krein trace formula. In [BS3] they used their approach under more restrictive assumptions on  $f$ .

*Proof.* Obviously,  $f$  is a Lipschitz function. As we have mentioned in the introduction,  $f$  is a differentiable function at every point of  $\mathbb{R}$  (but not necessarily continuously differentiable!). Put  $K \stackrel{\text{def}}{=} B - A$ . Consider the parametric family  $\{A_t\}_{0 \leq t \leq 1}$ ,  $A_t \stackrel{\text{def}}{=} A + tK$ . Then  $A_0 = A$  and  $A_1 = B$ . The operator  $K$  obviously belongs to the Hilbert–Schmidt class  $\mathcal{S}_2$ . As we have mentioned in § 3, the function

$t \mapsto f(A_t) - f(A)$  is differentiable in the Hilbert–Schmidt norm and

$$Q_t \stackrel{\text{def}}{=} \frac{d}{ds} (f(A_s) - f(A)) \Big|_{s=t} = \iint_{\mathbb{R} \times \mathbb{R}} \frac{f(x) - f(y)}{x - y} dE_t(x) K dE_t(y) \in \mathbf{S}_2,$$

where  $E_t$  is the spectral measure of  $A_t$ .

On the other hand, since the divided difference  $\mathfrak{D}f$  is a Schur multiplier of  $\mathbf{S}_1$  (see the introduction), it follows that

$$Q_t \in \mathbf{S}_1, \quad 0 \leq t \leq 1, \quad \text{and} \quad \sup_{t \in [0,1]} \|Q_t\|_{\mathbf{S}_1} < \infty.$$

We have

$$f(A) - f(B) = - \int_0^1 Q_t dt,$$

where the integral on the right is understood in the sense of Bochner in the space  $\mathbf{S}_1$ . It follows that

$$\text{trace} (f(A) - f(B)) = - \int_0^1 \text{trace}(Q_t) dt.$$

Since the function  $f$  is differentiable everywhere, the divided difference  $\mathfrak{D}f$  is continuous in each variable. By Theorem 5.1,

$$\text{trace} Q_t = \int_{\mathbb{R}} f'(x) d\nu_t(x),$$

where the signed measure  $\nu_t$  is defined by

$$\nu_t(\Delta) \stackrel{\text{def}}{=} \text{trace} (E_t(\Delta) K) \quad \text{for a Borel subset } \Delta \text{ of } \mathbb{R}.$$

We identify here the space of complex Borel measures on  $\mathbb{R}$  with the dual space to the Banach space of continuous functions on  $\mathbb{R}$  with zero limit at infinity. Then the function  $t \mapsto \nu_t$  is continuous in the weak-\* topology on the space of complex Borel measures. Indeed, if  $h$  is continuous on  $\mathbb{R}$  and  $\lim_{|x| \rightarrow \infty} h(x) = 0$ , then

$$\int h d\nu_t = \text{trace} (h(A_t) K).$$

The function  $t \mapsto h(A_t)$  is a continuous function on  $[0, 1]$  in the operator norm; this follows from the fact that  $h$  is an operator continuous function (see [AP1, § 8]). Thus the function  $t \mapsto \text{trace} (h(A_t) K)$  is continuous.

Therefore we can define the signed Borel measure  $\nu$  on  $\mathbb{R}$  by

$$\nu = \int_0^1 \nu_t dt.$$

It follows that

$$\text{trace} (f(A) - f(B)) = - \int_{\mathbb{R}} f' d\nu.$$

On the other hand, for smooth functions  $g$  with compact support,

$$\text{trace} (g(A) - g(B)) = \int_{\mathbb{R}} g' \xi dm,$$

where  $\xi$  is the spectral shift function.

It follows that  $\nu$  is absolutely continuous with respect to Lebesgue measure and  $d\nu = -\xi dm$ . □

Theorem 6.1 implies the following result:

**Theorem 6.2.** *Let  $f$  be an operator Lipschitz function and let  $A$  and  $B$  be self-adjoint operators such that  $A - B \in \mathcal{S}_1$ . Then the function*

$$t \mapsto \text{trace} (f(A - tI) - f(B - tI)), \quad t \in \mathbb{R},$$

*is continuous on  $\mathbb{R}$ .*

*Proof.* Consider the function  $f_t$ ,  $t \in \mathbb{R}$ , defined by  $f_t(x) \stackrel{\text{def}}{=} f(x - t)$ . Let  $\xi$  be the spectral shift function associated with  $(A, B)$ . It is easy to see that

$$\text{trace} (f(A + tI) - f(B + tI)) = \text{trace} (f_t(A) - f_t(B)) = \int_{\mathbb{R}} f'(x - t)\xi(x) dm(x),$$

which depends on  $t$  continuously.  $\square$

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