PUBLICATIONS DE L'INSTITUT MATHÉMATIQUE
Nouvelle série tome 54 (68), 1993, 71–79

TRACE FORMULA FOR NONNUCLEAR PERTURBATIONS OF SELFADJOINT OPERATORS

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Abstract. The trace formulas for the operator $\varphi(H_1)-\varphi(H_0)$ are deduced when H_1-H_0 is a nonnuclear operator and φ is an enough wide class of functions.

1. Introduction. Suppose $B(\mathcal{H})$ is the algebra of all bounded operators over the Hilbert space $\mathcal{H}$. Denote by C_p and $|\cdot|_p$ the Neumann-Schatten class of operators and their norm [**2**]. For an operator $W \in C_2$ by $\det_2(I+W)$ we denote its regularized determinant.

Let H_1 and H_0 be selfadjoint operators (possibly unbounded) on a Hilbert space $\mathcal{H}$. If $H_1-H_0=V$ is a nuclear operator and φ is an element in a sufficiently large class of functions, then Krein [**3,4**] proved that $\varphi(H_1)-\varphi(H_0)$ is a nuclear operator and that

$$\operatorname{trace}\left(\varphi\left(H_1\right)-\varphi\left(H_0\right)\right)=\int_R \xi(\lambda)\varphi'(\lambda)d\lambda, \tag{1.1}$$

where ξ is the real function in $L^1(R)$ uniquely determined by H_0 and H_1. Usually, the relation (1.1) is called the trace formula.

Krein also proved the following relation between the function and the perturbation determinant:

$$\det\left(I+V(H_0-z)^{-1}\right)=\exp\left(\int_R \frac{\xi(\lambda)}{\lambda-z}d\lambda\right), \quad \operatorname{Im} z\neq 0.$$

Koplienko [**5**] extended the trace formula (1.1) to the case when H_1-H_0 is not a nuclear operator. The trace formula was deduced when φ is a rational function with the poles in $C\backslash R$ and $|\varphi(\infty)|<\infty$.

AMS Subject Classification (1990): Primary 47 A 55

In this paper we prove regularized trace formulas for a nonnuclear perturbation of selfadjoint operators in the case when φ is not an analytic function. Our method is different from the method given in [**6**]. The following theorem is a result of Koplienko:

THEOREM 1.1 *Let H_0, V be selfadjoint operators, $V \in C_2$ and let φ be a rational function with poles lying in $C\backslash R$ and $|\varphi(\infty)| < \infty$. Then*

(1) $R_2 = \varphi(H_0+V) - \varphi(H_0) - \frac{d}{dx}\varphi(H_0+xV)|_{x=0} \in C_1$

(2) *There exists a real function σ (depending only on H_0 and V) of bounded variation such that*

$$\operatorname{trace} R_2 = \int\limits_R \varphi''(\lambda) d\sigma(\lambda)$$

(3) $V_{-\infty}^{\infty}\sigma \le |V|_2^2/2!$ *($V_{-\infty}^{\infty} f$ is the variation of f on $(-\infty,\infty)$).*

(4) $\det_2\left(I + V(H_0-z)^{-1}\right) = \exp\left(-\int\limits_R \frac{d\sigma(\lambda)}{(\lambda-z)^2}\right)$.

2. Results. Let $\mathcal{M}_p$ be the set of all the functions φ of the form $\varphi(x) = \int_R e^{itx} g(t) \mathrm{d}t$ where g is a measurable function such that $\int_R |t|^\nu |g(t)| dt < \infty$ for $\nu = 0,1,2,\dots p$ $(p \ge 2)$. The functions from $\mathcal{M}_p$ are not necessarily analytic, and the set $\mathcal{M}_p$ contains the class of functions from Theorem 1.

Recall that if $A, B \in B(\mathcal{H})$, then [**1**] we have

$$e^{(A+B)t} = e^{A\cdot t} + \sum_{n=1}^{\infty} \int_0^t \int_0^{s_1} \cdots \int_0^{s_{n-1}} e^{A(t-s_1)} B e^{A(s_1-s_2)} B \dots B e^{A(s_{n-1}-s_n)} B e^{As_n} ds_1 ds_2 \dots ds_n \tag{2.0.1}$$

(The series converges in $B(\mathcal{H})$).

LEMMA 2.1 *If $H_0 = H_0^*$, $V = V^* \in B(\mathcal{H})$, $t, x \in R$, then*

$$e^{it(H_0+xV)} = e^{itH_0} + \sum_{n=1}^{\infty} i^n x^n B_n(t), \tag{2.1.1}$$

where

$$B_n(t) = \int_0^t \int_0^{s_1} \cdots \int_0^{s_{n_1}} e^{iH_0(t-s_1)} V e^{iH_0(s_1-s_2)} V \dots V e^{iH_0(s_{n-1}-s_n)} V e^{iH_0 s_n} ds_1 ds_2 \dots ds_n \tag{2.1.2}$$

Proof. If $H_0 \in B(\mathcal{H})$, then (2.11) and (2.12) follow directly from (2.01). So, suppose that H_0 is an unbounded operator. Set $H^{(k)} = H_0 E(-k,k)$, where E is the spectral measure of H_0. The operator $H^{(k)}$ is bounded and we have

$$\lim_{k\to\infty} \left(\lambda - H^{(k)}\right)^{-1} h = (\lambda - H_0)^{-1} h \;\; (h \in \mathcal{H},\; \mathrm{Im}\lambda \neq 0)$$

i.e. the sequence $H^{(k)}$ converges to H_0 in the strong resolvent sense. By the Troter Theorem [**7**] we have

$$\lim_{k\to\infty} e^{itH^{(k)}}h = e^{itH_0}h, \quad h \in \mathcal{H}, \quad t \in R. \tag{2.1.3}$$

Setting $H^{(k)}$ instead of H_0 in (2.1.1), (2.1.2) and letting k tend to infinity, we complete the proof of Lemma 1.

LEMMA 2.2 *If* $H_0 = H_0^*$, $V = V^* \in B(\mathcal{H})$, $x, t \in R$, *then for* $k = 0, 1, 2, \ldots$ *the following inequality holds*

$$\left\| \frac{d^k}{dx^k} e^{it(H_0+xV)} \right\| \le |t|^k \|V\|^k. \tag{2.2.1}$$

Proof. Since

$$\frac{d^k}{dx^k} e^{it(H_0+xV)} = \frac{d^k}{d\xi^k} e^{it(H_1+\xi V)}|_{\xi=0} \left(H_1 = H_0 + xV\right),$$

by Lemma 2.1, it follows

$$\frac{d^k}{d\xi^k} e^{it(H_1+\xi V)}|_{\xi=0} = i^k k! \int_0^t \int_0^{s_1} \cdots \int_0^{s_{n-1}} e^{iH_1(t-s_1)} V \ldots V e^{iH_1 s_n} ds_1 ds_2 \ldots ds_n$$

From the previous equality we have

$$\left\| \frac{d^k}{dx^k} e^{it(H_0+xV)} \right\| \le k! \int_0^t \int_0^{s_1} \cdots \int_0^{s_{n-1}} \|V\|^k ds_1 ds_2 \ldots ds_n = |t|^k \|V\|^k, \ \ (t > 0)$$

and the proof is complete.

LEMMA 2.3 *If* $H_0 = H_0^*$, $x, t \in R$, $V = V^* \in B(\mathcal{H})$ *and* $\varphi \in \mathcal{M}_p$ *(i.e.* $\varphi(x) = \int_R e^{itx} g(t)dt$, *g is a measurable function), then*

$$\frac{d^k}{dx^k} \varphi\left(H_0 + xV\right) = \int_R \frac{d^k}{dx^k} e^{it(H_0+xV)} g(t)dt. \tag{2.3.1}$$

Proof. For $k = 0$, (2.3.1) follows from the spectral theorem. If $k = 1$ we have

$$\frac{d}{dx} \varphi\left(H_0 + xV\right) = \lim_{\xi\to\infty} \int_R \frac{e^{it(H_0+(x+\xi)V)} - e^{it(H_0+xV)}}{\xi} g(t)dt. \tag{2.3.2}$$

Since

$$e^{it(H_0+x_2V)} - e^{it(H_0+x_1V)} = \int_{x_1}^{x_2} \frac{\partial}{\partial x} e^{it(H_0+xV)} dx$$

by Lemma 2.2 we obtain

$$\left\|e^{it(H_0+x_2V)} - e^{it(H_0+x_1V)}\right\| \leq |t|\|V\||x_2 - x_1|. \tag{2.3.3}$$

From (2.3.2), (2.3.3) and $\int_R |t||g(t)|\mathrm{dt} < \infty$, by the Theorem of Dominated Convergence, we conclude that

$$\frac{d}{dx}\varphi\left(H_0 + xV\right) = \int\limits_R \frac{d}{dx}e^{it(H_0+xV)}g(t)dt.$$

Repeating this procedure several times we prove Lemma 2.3.

From now on we assume $V = V^* \in C_p$ $(p \geq 2,\ \ p \in N)$.

Lemma 2.4 *If $x, t \in R$, $H_0 = H_0^*$, then $\frac{d^p}{dx^p}e^{it(H_0+xV)}$ is a nuclear operator and*

$$\left|\frac{d^p}{dx^p}e^{it(H_0+xV)}\right|_1 \leq |t|^p|V|_p^p.$$

Proof. Since

$$\frac{d^p}{dx^p}e^{it(H_0+xV)} = i^p p! \int\limits_0^t \int\limits_0^{s_1} \cdots \int\limits_0^{s_{n-1}} e^{iH_1(t-s_1)}V \ldots Ve^{iH_1(s_{p-1}-s_p)}Ve^{iH_1 s_p}ds_1 ds_2 \ldots ds_n$$

$(H_1 = H_0 + xV)$ and $V \in C_p$ we get $\frac{d^p}{dx^p}e^{it(H_0+xV)} \in C_1$ and

$$\left|\frac{d^p}{dx^p}e^{it(H_0+xV)}\right| \leq p!|V|_p^p \int\limits_0^t \int\limits_0^{s_1} \cdots \int\limits_0^{s_{p-1}} ds_1 ds_2 \ldots ds_n = t^p|V|_p^p \ \ (t > 0).$$

Set

$$U_p(t) = e^{it(H_0+V)} - \sum_{k=0}^{p-1}\frac{1}{k!}\frac{d^k}{dx^k}e^{it(H_0+xV)}|_{x=0}$$

Now, by Lemma 2.3

$$R_p \stackrel{\text{def}}{=} \varphi\left(H_0 + V\right) - \sum_{k=0}^{p-1}\frac{1}{k!}\frac{d^k}{dx^k}\varphi\left(H_0 + xV\right)|_{x=0} = \int\limits_R U_p(t)g(t)dt.$$

Lemma 2.5 *If $H_0 = H_0^*$, $V = V^* \in C_p$, $t \in R$, then $U_p(t) \in C_1$, $R_p \in C_1$ and*

$$\operatorname{trace} R_p = \int\limits_R g(t)\ \ \operatorname{trace} U_p(t)\mathrm{dt} \tag{2.5.1}$$

Proof. Let $m(x) = e^{it(H_0+xV)}$, (where t is a fixed real number and $x \in R$). By the Teylor theorem we obtain

$$m(1) = \sum_{\nu=0}^{p-1} \frac{m^{(\nu)}(0)}{\nu!} + \frac{1}{(p-1)!} \int_0^1 m^{(p)}(x)(1-x)^{p-1} dx$$

i.e.

$$U_p(t) = \frac{1}{(p-1)!} \int_0^1 m^{(p)}(x)(1-x)^{p-1} dx$$

Since $m^{(p)}(x) \in C^1$ (by Lemma 2.4) and $m^{(p)}$ is a continuous function in C_1 norm, we have $U_p(t) \in C_1$ $(\forall t \in R)$. By Lemma 2.4 we get

$$|U_p(t)|_1 \leq \frac{1}{(p-1)!} \int_0^1 \left| m^{(p)}(x) \right|_1 (1-x)^{p-1} dx \leq \frac{1}{(p-1)!} \int_0^1 |t|^p |V|_p^p (1-x)^{p-1} dx$$

i.e.

$$|U_p(t)|_1 \leq |V|_p^p |t|^p / p!. \tag{2.5.2}$$

Hence R_p is a compact operator.

Let S be a unitary operator and suppose $\{e_i\}$ is an orthonormal set. Then

$$\begin{aligned} \left| \sum_{i=1}^{r} (SR_p e_i, e_i) \right| &= \left| \sum_{i=1}^{r} \left(\int_R g(t) SU_p(t) e_i, e_i \right) \right| = \left| \int_R g(t) \sum_{i=1}^{r} (SU_p(t) e_i, e_i)\, dt \right| \\ &\leq ([\mathbf{2}]) \leq \int_R |g(t)| \sum_{i=1}^{r} s_i\left(U_p(t)\right) dt \leq \int_R |g(t)| \left|U_p(t)\right|_1 dt \\ &\leq \int_R |g(t)| |t|^p dt \cdot \frac{|V|_p^p}{p!}. \qquad \text{(by 2.5.2)} \end{aligned}$$

So,

$$\left| \sum_{i=1}^{r} (SR_p e_i, e_i) \right| \leq \frac{|V|_p^p}{p!} \int_R |t|^p |g(t)| dt.$$

When we take the supremum over all unitary operators S and over all orthonormal sets $\{e_i\}$, we obtain

$$\sum_{i=1}^{r} s_i\left(R_p\right) \leq \frac{|V|_p^p}{p!} \int_R |t|^p |g(t)| dt,$$

i.e.

$$R_p \in C_1, \; |R_p|_1 \leq \frac{|V|_p^p}{p!} \int_R |t|^p |g(t)| dt \; \text{ and } \; \operatorname{trace} R_p = \int_R g(t) \; \operatorname{trace} U_p(t) dt.$$

This completes the proof

Lemma 2.6 *If* $H_0 = H_0^* \in B(\mathcal{H})$, $V = V^* \in C_p$ *and* $\Gamma = \{\lambda\colon |\lambda| = 1 + \|H_0\| + \|V\|\}$, *then*

$$U_p(t) = \frac{1}{2\pi i}\int_\Gamma e^{i\lambda t} G_p(\lambda)d\lambda$$

where $G_p(\lambda) = (\lambda - H_0)^{-1}(V(\lambda - H_0)^{-1})^p (I - V(\lambda - H_0)^{-1})^{-1}$

Proof. From $H_0 = H_0^*$ we have $\|V(\lambda - H_0)^{-1}\| \le \|V\|(1 + \|V\|)^{-1} < 1$ for every $\lambda \in \Gamma$. Hence $(\lambda - H_0 - xV)^{-1} = \sum_{k=0}^{\infty} x^k (\lambda - H_0)^{-1}(V(\lambda - H_0)^{-1})^k$; it follows that

$$\frac{d^k}{dx^k}(\lambda - H_0 - xV)^{-1}|_{x=0} = k!\,(\lambda - H_0)^{-1}\left(V(\lambda - H_0)^{-1}\right)^k$$

and

$$\frac{1}{k!}\frac{d^k}{dx^k} e^{it(H_0 + xV)}|_{x=0} = \frac{1}{2\pi i}\int_\Gamma e^{i\lambda t}(\lambda - H_0)^{-1}\left(V(\lambda - H_0)^{-1}\right)^k d\lambda \tag{2.6.2}$$

Since $e^{it(H_0+V)} = \frac{1}{2\pi i}\int_\Gamma e^{i\lambda t}(\lambda - H_0 - V)^{-1}d\lambda$ from (2.6.2) it follows

$$U_p(t) = \frac{1}{2\pi i}\int_\Gamma e^{i\lambda t}\sum_{k=p}^{\infty}(\lambda - H_0)^{-1}\left(V(\lambda - H_0)^{-1}\right)^k d\lambda = \frac{1}{2\pi i}\int_\Gamma e^{i\lambda t} G_p(\lambda)d\lambda$$

Lemma 2.7 *Let* $H_0 = H_0^*$ *be an unbounded operator and* $V = V^* \in C_p$. *If* $H_0^{(n)} = H_0 E(-n, n)$ *(E is the spectral measure of* H_0*) and*

$$U_p^{(n)}(t) = e^{it(H_0^{(n)} + V)} - \sum_{k=0}^{p-1}\frac{1}{k!}\frac{d^k}{dx^k} e^{it(H_0^{(n)} + xV)}|_{x=0}$$

then for every $t \in R$

$$\lim_{n\to\infty}\left|U_p(t) - U_p^{(n)}(t)\right|_1 = 0. \tag{2.7.1}$$

Proof. Since

$$U_p(t) = \frac{1}{(p-1)!}\int_0^1 m^{(p)}(x)(1-x)^{p-1}dx$$

and

$$U_p^{(n)}(t) = \frac{1}{(p-1)!}\int_0^1 m_n^{(p)}(x)(1-x)^{p-1}dx$$

where $m(x) = e^{it(H_0+xV)}$ and $m_n(x) = e^{it(H_0^{(n)}+xV)}$, we obtain

$$\left|U_p(t) - U_p^{(n)}(t)\right|_1 \le \frac{1}{(p-1)!}\int_0^1 \left|m^{(p)}(x) - m_n^{(p)}(x)\right|_1 (1-x)^{p-1}dx$$

From (2.1.1), (2.1.2) and [**2**, p. 119], Theorem 6.3 we have

$$\lim_{n\to\infty}\left|m^{(p)}(x) - m_n^{(p)}(x)\right|_1 = 0,\ \ x \in (0,1).$$

Now, since $\left|m^{(p)}(x)\right|_1 \le |t|^p|V|_p^p$ and $\left|m_n^{(p)}(x)\right|_1 \le |t|^p|V|_p^p$, (2.7.1) follows from the Lebesgue Dominated Convergence Theorem.

THEOREM 2.8 *If $V \in C_2$, $H_0 = H_0^*$ and $\varphi \in \mathcal{M}_2$, then*

(1) $R_2 = \varphi(H_0+V) - \varphi(H_0) - \frac{d}{dx}\varphi(H_0+xV)|_{x=0} \in C_1$

(2) *There exists a real function σ of bounded variation (σ depends only on H_0 and V) such that trace $R_2 = \int_R \varphi''(\lambda)d\sigma(\lambda)$*

(3) $V_{-\infty}^{\infty}\sigma \le |V|_2^2/2$

(4) $\det_2\left(I + V(H_0-z)^{-1}\right) = \exp\left(-\int\limits_R \frac{d\sigma(\lambda)}{(\lambda-z)^2}\right).$

Proof. (1) follows from Lemma 2.5. Let H_0 be a bounded operator, $\lambda_0 \in C\backslash R$ and $|\lambda_0| > 1 + \|H_0\| + \|V\|$. Now, by Runge's Theorem there exists a sequence of polinomials P_n such that $r_n(\lambda) := P_n(1/(\lambda-\lambda_0)) \rightrightarrows e^{i\lambda t}$ on $D = \{\lambda : |\lambda| \le 1 + \|H_0\| + \|V\|\}$. Hence

$$r_n^{(\nu)}(\lambda) \rightrightarrows (it)^\nu e^{it}\lambda\ \ (\nu = 0,1,2,\dots)\ \text{on}\ D. \tag{2.8.1}$$

Let $R_2^{(n)} = r_n(H_0+V) - r_n(H_0) - \frac{d}{dx}r_n(H_0+xV)|_{x=0}$. As in Lemma 2.6, we get

$$R_2^{(n)} = \frac{1}{2\pi i}\int_\Gamma r_n(\lambda)G_2(\lambda)d\lambda.$$

Now, by Lemma 2.6 we have

$$U_2(t) - R_2^{(n)}(t) = \frac{1}{2\pi i}\int_\Gamma \left(e^{i\lambda t} - r_n(\lambda)\right)G_2(\lambda)d\lambda$$

and

$$\left|U_2(t) - R_2^{(n)}(t)\right|_1 \le \frac{1}{2\pi}\int_\Gamma \left|e^{i\lambda t} - r_n(\lambda)\right| \cdot \max_{\lambda\in\Gamma}|G_2(\lambda)|_1 \cdot |d\lambda| \longrightarrow 0\ \ (n\to\infty).$$

Hence $\lim_{n\to\infty}\operatorname{trace} R_2^{(n)} = \operatorname{trace} U_2(t)$. By Theorem 1, there exists a function σ of bounded variation (depending only on H_0 and V) such that $V_{-\infty}^{\infty}\sigma \le |V|_2^2/2!$ and

$$\operatorname{trace} R_2^{(n)} = \int_R r_n''(s)d\sigma(s) \tag{2.8.2}$$

From (2.8.1) and (2.8.2) it follows

$$\operatorname{trace} U_2(t) = \int_R (it)^2 e^{its} d\sigma(s). \tag{2.8.3}$$

From (2.5.1) and (2.8.3) we conclude trace $R_2 = \int_R \varphi''(s) d\sigma(s)$.

Now consider the case when H_0 is not a bounded operator. Lemma 2.7 gives

$$\lim_{n\to\infty} \operatorname{trace} U_2^{(n)}(t) = \operatorname{trace} U_2(t). \tag{2.8.4}$$

From (2.8.3) it follows

$$\operatorname{trace} U_2^{(n)}(t) = \int_R (it)^2 e^{\mathrm{its}} d\sigma_n(s) \text{ and } V_{-\infty}^{\infty}\sigma_n \leq \frac{|V|_2^2}{2!}.$$

By (2.8.4) and the Helly election Theorem there exists a function σ of bounded variation $\left(V_{-\infty}^{\infty}\sigma \leq |V|_2^2/2!\right)$ such that

$$\operatorname{trace} U_2(t) = \int_R (it)^2 e^{its} d\sigma(s) \text{ and } \operatorname{trace} R_2 = \int_R \varphi''(s) d\sigma(s).$$

The property (4) we obtain similarly as in [**5**].

THEOREM 2.9 *If $H_0 = H_0^* \in B(\mathcal{H})$, $V = V^* \in C_p$ ($p \geq 3$, $p \in N$) and $\varphi \in \mathcal{M}_{p+1}$, then*

$$\operatorname{trace} R_p = \frac{\operatorname{trace} V^p}{p!}\varphi^{(p)}(0) + \int_R \varphi^{(p+1)}(x)\gamma(x)dx$$

where $\gamma \in L^2(R)$ is a function which depends only on V, H_0 and p.

Proof. From Lemma 2.6 it follows that $f(t) = \operatorname{trace} U_p(t)$ is an entire function of the exponential type. On the other hand from (2.5.2) we get $|f(t)| \leq |t|^p |V|_p^p/p!$ for every $t \in R$. Hence $f(0) = f'(0) = \cdots = f^{(p-1)}(0) = 0$. From (2.6.1) we obtain

$$\lim_{t\to 0} \frac{f(t)}{(it)^p} = \frac{\operatorname{trace} V^p}{p!}$$

So, $\frac{1}{t}\left(\frac{f(t)}{(it)^p} - \frac{\operatorname{trace} V^p}{p!}\right) \in L^2(R)$ is an entire function of the exponential type. Now, by the Paley-Wiener Theorem we have

$$\frac{f(t)}{(it)^p} - \frac{\operatorname{trace} V^p}{p!} = it \int_R e^{its}\gamma(s)ds$$

for some $\gamma \in L^2(R)$ and

$$f(t) = (it)^{p+1}\int_R e^{its}\gamma(s)ds + (it)^p \frac{\operatorname{trace} V^p}{p!}. \tag{2.9.1}$$

The proof of Theorem 2.9 follows from (2.5.1) and (2.9.1).

COROLLARY 2.10. *If $H_0 = H_0^*$ is an unbounded operator, $V = V^* \in C_p$ $(p \geq 3)$, then there exists a sequence $\gamma_n \in L^2(R)$ such that for every $\varphi \in \mathcal{M}_{p+1}$*

$$\operatorname{trace} R_p = \frac{\operatorname{trace} V^p}{p!}\varphi^{(p)}(0) + \lim_{n\to\infty}\int_R \varphi^{(p+1)}(x)\gamma_n(x)dx.$$

Proof. Since

$$R_p^{(n)} = \varphi\left(H_0^{(n)} + V\right) - \sum_{k=0}^{p-1}\frac{1}{k!}\frac{d^k}{dx^k}\varphi\left(H_0^{(n)} + xV\right)|_{x=0}\left(H_0^{(n)} = H_0 E\left(-n,n\right)\right)$$
$$= \int_R g(t)U_p^{(n)}(t)dt,$$

by Lemma 2.7 we get

$$\lim_{n\to\infty} \operatorname{trace} R_p^{(n)} = \operatorname{trace} R_p. \qquad (2.10.1)$$

By Theorem 2.9 there exists a sequence $\gamma_n \in L^2(R)$ such that

$$\operatorname{trace} R_p^{(n)} = \frac{\operatorname{trace} V^p}{p!}\varphi^{(p)}(0) + \int_R \varphi^{(p+1)}(x)\gamma_n(x)dx$$

and the proof follows by (2.10.1).

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(Received 28 06 1993)
(Revised 17 03 1994)