Indag. Mathem., N.S., 20 (3), 477–482 September 2009

by Rein Zeinstra

Osterstrasse 8, 20259 Hamburg, Germany

Communicated by Prof. J. Korevaar

ABSTRACT

This note shows that a certain identity for the spectral function of one-particle states, known as the sum rule in Quantum Statistical Mechanics, holds true for a rather wide class of non-negative functions on the real line.

1. INTRODUCTION AND MAIN RESULT

For certain non-negative functions u on the real line corresponding to lifetime decay of one-particle states in Quantum Statistical Mechanics (QSM) one has on physical grounds the "spectral" identity

$$(1.1)\qquad \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{u(x)}{u(x)^2+(x-\tilde{u}(x))^2}\,dx = 1.$$

This so-called "sum rule" appears for example in the book of Kadanoff–Baym [3] in the form $\frac{1}{2\pi}\int_{-\infty}^{\infty} A(p,\omega)\,d\omega = 1$ ([3], p. 8/29). The integrand of (1.1) is called the spectral function in QSM. The function $\tilde{u}$ appearing in it denotes the Hilbert transform of u. It is defined by the Cauchy principal value integral

$$(1.2)\qquad \tilde{u}(x) := \frac{1}{\pi}\mathrm{PV}\int_{-\infty}^{\infty} \frac{u(t)}{x-t}\,dt.$$

E-mail: rl.zeinstra@googlemail.com (R. Zeinstra).

In order for the right-hand side of (1.2) to make sense it must be assumed (for $u \geqslant 0$) that

$$\int_{-\infty}^{\infty} \frac{u(t)}{|t|+1}\,dt < \infty. \tag{1.3}$$

Under this condition the singular integral in (1.2) is known to exist finitely for almost every (a.e.) x.

In view of its importance for QSM it is natural to investigate for which non-negative functions u subject to (1.3) the identity (1.1) holds. In [4] Koehler conjectured that (1.1) would hold for "all" functions u. Koehler's conjecture was noticed by Kondratyev and henceforth answered in the negative in [1]. In a later paper [6] it was shown that each (strictly positive) function u, whose reciprocal u^{-1} is locally bounded and which belongs to some space L^p with $1 < p < \infty$, satisfies (1.1). In fact, in [6] it was shown that (1.1) under the given conditions could be obtained as a limiting case of Cauchy's theorem when the bounding contour is moved to infinity. The boundedness condition $u \in L^p$ in that paper allowed to apply a classical theorem of Marcel Riesz stating that the Hilbert transform $u \mapsto \tilde{u}$ is bounded on L^p $(1 < p < \infty)$. This fact was then used to carry out the delicate limiting process in the application of Cauchy's theorem.

In the present paper the condition $u \in L^p$ is removed altogether. Our new proof avoids the use of Cauchy's theorem. It requires only (1.3), or the even weaker condition (for an analogue of (1.1))

$$\int_{-\infty}^{\infty} \frac{u(t)}{t^2+1}\,dt < \infty. \tag{1.4}$$

We also substantially weaken the condition that u locally have a positive lower bound, replacing it by the more natural condition $u^{-1} \in L^1_{\mathrm{loc}}$. (As a matter of fact, QSM does not forbid the lifetime decay function u to be zero at an isolated value of the argument.) The condition is sharp as an explicit counterexample in [6] with u a C^∞-function with a single zero shows. Our main result is the following theorem.

Theorem 1. *Let u be a non-negative locally integrable function satisfying* (1.3) *and let $\tilde{u}$ be its Hilbert transform given by* (1.2). *Let furthermore a, b be arbitrary real numbers, $a > 0$. Then we have the inequality*

$$\int_{-\infty}^{\infty} \frac{u(x)}{u(x)^2 + (\tilde{u}(x) - ax - b)^2}\,dx \leqslant \frac{\pi}{a}. \tag{1.5}$$

If moreover, $1/u(x)$ be locally integrable then equality holds in (1.5)*:*

$$\int_{-\infty}^{\infty} \frac{u(x)}{u(x)^2 + (\tilde{u}(x) - ax - b)^2}\,dx = \frac{\pi}{a}. \tag{1.6}$$

In the QSM-interpretation of this theorem the variable of integration x corresponds to energy. (Under the normalizations $a = 1, h/2\pi = 1$, where h is Planck's constant.) The function u characterizes lifetime while its Hilbert transform $\tilde{u}$ represents the correlation part of interacting energy; the constant b represents the energy of a particle in the Hartree–Fock approximation (cf. [3]).

In one sense Theorem 1 can still not be considered as being optimal. For example (1.3) still requires $u(t)$ to tend to 0 at $\pm\infty$, at least on average. In particular, while all spaces L^p, $1 \leqslant p < \infty$, are included, simple bounded functions like the (positive) constants are not! In section 3 we shall consider an extension of Theorem 1 with (1.3) replaced by the weaker condition (1.4).

2. PROOF OF THEOREM 1

We shall modify the proof of [6]. In the following all integrals will be over the whole real axis. First let us recall a few well-known facts. (See e.g. Koosis [5].) Let $U = \mathrm{P}u$ denote the Poisson integral of u in the upper half-plane $z = x + \mathrm{i}y$, $y > 0$:

$$U(z) = \frac{y}{\pi} \int \frac{u(t)}{(x-t)^2 + y^2}\, dt. \tag{2.1}$$

Then $U(z)$ is a positive harmonic function, $U(x + \mathrm{i}y) \to u(x)$ a.e. (Fatou's theorem) and in $L^1_{\mathrm{loc}}(\mathbb{R})$ as $y \downarrow 0$. Also $U = \operatorname{Re} H$, where

$$H(z) = \frac{\mathrm{i}}{\pi} \int \frac{u(t)}{z - t}\, dt \tag{2.2}$$

is holomorphic in the half-plane $y > 0$. Putting $\tilde{U} = \operatorname{Im} H$ we have

$$\tilde{U}(z) = \frac{1}{\pi} \int \frac{(x-t)u(t)}{(x-t)^2 + y^2}\, dt \tag{2.3}$$

and $\tilde{U}(x + \mathrm{i}y) \to \tilde{u}(x)$ a.e.

After these preliminaries we begin with the actual proof. We may assume that $a = 1$, by a change of scale. We further note that the reciprocal function $H(z)^{-1}$ also has positive real part in the upper half-plane. Replacing $H(z)$ by $H(z) - \mathrm{i}(z + b)$ – which increases its real part – and putting $T(z) := (H(z) - \mathrm{i}(z + b))^{-1}$, $S(z) := \operatorname{Re} T(z)$, we then have

$$S(z) = \frac{U(z) + y}{(U(z) + y)^2 + (\tilde{U}(z) - x - b)^2}, \qquad y > 0. \tag{2.4}$$

We conclude that $S(x + \mathrm{i}y) \to s(x)$ a.e., where s is the spectral function, i.e. the integrand of (1.6) (with $a = 1$).

We now note that according to the classical Riesz–Herglotz Theorem (cf. [5]) we can write each positive harmonic function V in the upper half-plane in a unique way in the form $V = \mathrm{P}\mu + ky$, where $\mathrm{P}\mu$ denotes the Poisson integral of a non-negative Borel measure μ satisfying

$$\int \frac{d\mu(t)}{t^2 + 1} < \infty \tag{2.5}$$

and k a non-negative constant. Moreover, $V(x+\mathrm{i}y) \to \mu$ weak* as $y \downarrow 0$ (that is, $\int f(x)V(x+\mathrm{i}y)\,dx \to \int f(x)\,d\mu(x)$ for all continuous f of compact support) and $V(x+\mathrm{i}y) \to v(x)$ a.e. (Fatou), where v is the Radon–Nikodym derivative of the absolutely continuous part μ_a in the Lebesgue decomposition $\mu = \mu_a + \mu_s$. Moreover, $V(x+\mathrm{i}y) \to v(x)$ in L^1_{loc} if and only if the singular part μ_s vanishes, i.e. if μ is absolutely continuous with density v. Applying this with $V = S, v = s$ we obtain

$$S(z) = \frac{y}{\pi}\int \frac{d\mu(t)}{(x-t)^2+y^2} + ky, \quad y > 0, \tag{2.6}$$

where $d\mu_a(x) = s(x)\,dx$. In particular,

$$\int s(x)\,dx \leqslant \mu(\mathbb{R}), \tag{2.7}$$

with equality if and only if μ is absolutely continuous.

Now a simple application of Lebesgue's dominated convergence theorem using the convergence condition (2.5) shows that $\mathrm{P}\mu(\mathrm{i}y)/y \to 0$ as $y \to \infty$. Thus the constant k in (2.6) is determined by $k = \lim S(\mathrm{i}y)/y$. Another application of Lebesgue's theorem using condition (1.3) shows that $H(\mathrm{i}y)/y \to 0$, i.e. both $U(\mathrm{i}y)/y \to 0$ and $\tilde{U}(\mathrm{i}y)/y \to 0$ as $y \to \infty$.

From this and (2.4) we conclude that $yS(\mathrm{i}y) \to 1$. In particular, the constant k must be 0. We can now apply Lebesgue's *monotone* convergence theorem to the integral in (2.6) to obtain $yS(\mathrm{i}y) \to \mu(\mathbb{R})/\pi$. It follows that μ is a finite measure, $\mu(\mathbb{R}) = \pi$. With (2.7) this proves (1.5). And (1.6) will follow if we can show that μ must be absolutely continuous if, in addition, u^{-1} be locally integrable. By the above remarks on the Riesz–Herglotz theorem we therefore have to show that $S(x+\mathrm{i}y) \to s(x)$ in L^1_{loc}. We need the following lemma.

Lemma 1. *Let u and U be as before, $u^{-1} \in L^1_{\mathrm{loc}}$. Let $R > 0$ be arbitrary and let $V = V_R$ be the Poisson integral of the function $v = v_R$ given as the restriction of u^{-1} to the interval $[-R, R]$ (and equal to zero otherwise). Then the following estimate holds:*

$$\left(\frac{1}{\pi}\arctan\frac{R}{y}\right)^2 \leqslant U(z)V(z), \quad |x| \leqslant R, y > 0. \tag{2.8}$$

In particular,

$$16U(z)V(z) \geqslant 1, \quad |x| \leqslant R, 0 < y \leqslant R. \tag{2.9}$$

Proof. Given any non-negative functions f, g on $\mathbb{R}$ the Schwarz inequality gives $(\mathrm{P}(fg))^2 \leqslant \mathrm{P}f^2 \cdot \mathrm{P}g^2$. We apply this with $f = \sqrt{u}$, $g = \sqrt{v}$. (The choice $g = 1/\sqrt{u}$ does not work since in general $\mathrm{P}u^{-1} \equiv \infty$.) Thus fg is the indicator function of the interval $[-R, R]$. For $x = \operatorname{Re} z$ restricted to the interval $[-R, R]$ one easily obtains (cf. (2.1), u replaced by fg), the estimate $\mathrm{P}(fg) \geqslant 1/\pi \cdot \arctan R/y$. The lemma follows. □

Combining now identity (2.4) and estimate (2.9) we obtain

$$(2.10) \qquad S(z) \leqslant U(z)^{-1} \leqslant 16V(z), \qquad |x| \leqslant R, 0 < y < R.$$

Since $V = \mathrm{P}v$, we have $V(x+\mathrm{i}y) \to v(x) = u^{-1}(x)$ in L^1 on $[-R, R]$. In connection with (2.10) this would imply *locally uniform integrability* of the family $S(x+\mathrm{i}y)$ and allow the conclusion that $S(x+\mathrm{i}y) \to s(x)$ in L^1 on $[-R, R]$ from Vitali's extension of Lebesgue's dominated convergence theorem. However, it is possible to use instead a much simpler extension of Lebesgue's theorem, contained in the following lemma.

Lemma 2 (cf. Elstrodt [2]). *Let ν be a measure on a measure space X. Let f_n be a sequence in $L^1(\nu)$ which converges pointwise to a function f on X. Suppose there exist functions g_n, g in $L^1(\nu)$ satisfying $|f_n| \leqslant g_n$, $g_n \to g$ pointwise, $\int_X g_n \, d\nu \to \int_X g \, d\nu$. Then $f \in L^1(\nu)$ and $f_n \to f$ in $L^1(\nu)$.*

Proof. Fatou's lemma applied to the non-negative (!) sequence $h_n(z) := g_n + g - |f_n - f|$. □

We apply Lemma 2 (with *continuous* parameter y) with ν equal to Lebesgue measure on $X = [-R, R]$, with $S(x+\mathrm{i}y), s(x)$ in the role of f_n, f, and finally with $V(x+\mathrm{i}y), v(x) = u(x)^{-1}$ in the role of g_n, g. This gives $S(x+\mathrm{i}y) \to s(x)$ for $y \downarrow 0$ in $L^1([-R, R])$. Since $R > 0$ is arbitrary, we conclude that the measure μ in (2.6) is absolutely continuous. Consequently identity (1.6) holds.

3. EXTENSION OF THE RESULT

From the point of view of QSM it is desirable that the class of admissible input functions u contain also certain slowly growing functions like $u(x) = |x|^\alpha$, $0 \leqslant \alpha < 1$. For such special *even* functions the Hilbert transform $\tilde{u}$ can still be defined by (1.2) if we interpret the integral appearing in it as a Cauchy principal value not only at $t = x$, but also for t at infinity. Similarly for (2.2) and (2.3). For example, if $u \equiv 1$ we would get $\tilde{u} \equiv 0$ and the identity (1.6) would simply become the statement that the standard Poisson kernel has total integral 1. Likewise, direct calculation would show validity of (1.6) for $u(x) = |x|^\alpha$, $0 < \alpha < 1$. (Cf. [1] for the case $\alpha = 1/2$.)

In this section we briefly describe how to extend Theorem 1 to the *whole* class of functions u satisfying (1.4). This is the class of (non-negative) functions u for which the Poisson integral U can be defined by (2.1). The definitions (1.2) and (2.2) in general no longer make sense, but we can modify them as follows: given any $\alpha > 0$ we define

$$\tilde{u}_\alpha(x) = \frac{1}{\pi} \mathrm{PV} \int u(t) \left(\frac{1}{x-t} + \frac{t}{t^2 + \alpha^2} \right) dt.$$

The modified kernel in brackets on the right is $O(t^{-2})$, so there is no longer a convergence problem at $\pm\infty$. Likewise we define

$$H_\alpha(x) = \frac{\mathrm{i}}{\pi} \int u(t) \left(\frac{1}{z-t} + \frac{t}{t^2+\alpha^2} \right) dt$$

(so that still $U = \operatorname{Re} H_\alpha$), and we put $\tilde{U}_\alpha := \operatorname{Im} H_\alpha$. (This modified harmonic conjugate of U vanishes at $i\alpha$, cf. (2.3). Our original harmonic conjugate corresponds to $\alpha = \infty$.) Naturally, $\tilde{U}_\alpha(x+\mathrm{i}y) \to \tilde{u}_\alpha(x)$ a.e. and the proof in Section 2 goes through as before. (In particular we have $H_\alpha(\mathrm{i}y)/y \to 0$ as $y \to \infty$, just as before for H.) So Theorem 1 remains true when $\tilde{u}$ is replaced by any $\tilde{u}_\alpha$.

The case of even functions u mentioned at the beginning of this section deserves special interest. Here all $\tilde{u}_\alpha$ coincide – as do all $\tilde{U}_\alpha$, H_α; indeed, because of oddness of the kernel they vanish identically on the positive imaginary axis. The resulting quasi-canonical $\tilde{u}$ coincides with the “double” principal value integral mentioned before.

ACKNOWLEDGEMENTS

It is a pleasure to recognize my indebtedness to Professors Alexander Kondratyev and Alexander Alenitsyn for communicating this interesting problem to me and for explaining its quantum mechanical background.

I also wish to express my gratitude to the Abdus Salam School of Mathematical Sciences in Lahore for its hospitality during stays in Autumn 2008 and Spring 2009, giving me optimal opportunity for helpful discussions on the present subject with Professors Kondratyev and Alenitsyn.

REFERENCES

[1] Alenitsyn A., Arshad M., Kondratyev A., Siddique I. – Hilbert transform: A new integral formula, in: Physics at Schools and Universities, Intern. Collection of Scientific Articles, Issue 7, Library Russ. Acad. Sci., St. Petersburg, 2007, pp. 3–7.

[2] Elstrodt J. – Maß- und Integrationstheorie, 2nd edn, Springer, Berlin, 1999.

[3] Kadanoff L.P., Baym G. – Quantum Statistical Mechanics, Benjamin, New York, NY, 1962 (Perseus Book, Cambridge, MA, 1989).

[4] Koehler H.S. – Phys. Rev. **46** (1992) 1687.

[5] Koosis P. – Introduction to H^p spaces, 2nd edn, Cambridge University Press, 1998.

[6] Zeinstra R., Alenitsyn A., Arshad M. – Identity for a spectral function connected with the Hilbert transform, J. Math. Sciences **150** (2008) 1799–1806 (Russian original in: Problems in Math. Anal. **36** (2007), 23–28).

(Received October 2009)