Assorted Problems

Various Authors

1. Preservation of bandlimitedness under non-affine time warping for multi-dimensional functions

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If $f \in L^2(\mathbf{R}^d)$ has compactly supported Fourier transform and $\gamma : \mathbf{R}^d \to \mathbf{R}^d$ has the form $\gamma(x) = Ax + b$ where $A \in GL_d(\mathbf{R})$ and $b \in \mathbf{R}^d$, then $h = f \circ \gamma$ also has compactly supported Fourier transform. It is possible to construct specific f and γ so that f and $f \circ \gamma$ both have compactly supported Fourier transforms, f is not the zero function, and γ is a continuous and invertible function that is not of the affine form just given. This construction can be accomplished, for example, by considering a d-fold cartesian product of known one-dimensional examples such as described in [1].

Under the assumption that $\gamma : \mathbf{R}^d \to \mathbf{R}^d$ is continuous and invertible, is it true that $f \circ \gamma$ has compactly supported Fourier transform for all $f \in L^2(\mathbf{R}^d)$ with compactly supported Fourier transform if and only if $\gamma(x) = Ax + b$?

[1] D. Cochran, S. Azizi, and J.N. McDonald, "Harmonic analysis and sampling in warped spaces," in *20th Century Harmonic Analysis — A Celebration*, J.S. Byrnes, ed.

2. Window pairs that determine spectral phase

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Consider a finite sequence

$$a(0),\ a(1),\ ...,\ a(n) \tag{2.1}$$

of complex numbers and the associated polynomial

$$p(z) = a(0) + a(1)z + \cdots + a(n)z^n. \tag{2.2}$$

The *spectral magnitude* of the sequence (2.1) or its associated polynomial (2.2) is the function $s : \mathbf{R} \to \mathbf{C}$ defined by $s(\omega) = |p(e^{i\omega})|$. In general, it is clear that two different polynomials can have identical spectral magnitude functions. If, however, two polynomials $p(z)$ and $q(z)$ have identical spectral magnitude functions *and* their respective derivatives $p'(z)$ and $q'(z)$

also have identical spectral magnitude functions (i.e., $|p'(z)| = |q'(z)|$ for all z with $|z| = 1$), then it can be shown that $p(z) = cq(z)$ for some complex constant c with $|c| = 1$.

Define finite sequences $w_1(k) = 1$ and $w_2(k) = k$ for $k = 0, ..., n$ and consider the sequences $b_1(k) = a(k)w_1(k)$ and $b_2(k) = a(k)w_2(k)$ obtained by "windowing" the original sequence $a(0), ..., a(n)$ with each of these new sequences. The polynomial associated with $b_2(0), ..., b_2(n)$ is $r(z) = zp'(z)$, which has spectral magnitude function identical to that of $p'(z)$. Hence, the spectral magnitude functions of the two windowed sequences are sufficient to determine $p(z)$ up to a unimodular constant factor.

The problem posed here is to characterize all pairs of window sequences $w_1(0), ...w_1(n)$ and $w_2(0), ...w_2(n)$ with the property that the spectral magnitude functions of the sequences $b_1(k) = a(k)w_1(k)$ and $b_2(k) = a(k)w_2(k)$ are sufficient to determine any polynomial $p(z)$ of degree n up to a unimodular constant factor. The corresponding problem with spectral phase in place of spectral magnitude is also of interest.

3. Questions on Riesz Products

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Riesz products, identified with positive measures, are of the form

$$\begin{aligned} \mu_a &= \prod_{n=1}^{\infty} \left(1 + \Re(a_n e^{i\lambda_n x})\right) \\ \mu_b &= \prod_{n=1}^{\infty} \left(1 + \Re(b_n e^{i\lambda_n x})\right) \end{aligned}$$

where (λ_n) is a given Hadamard sequence ($\lambda_1 > 0$, $\frac{\lambda_{n+1}}{\lambda_n} > q > 1$), $a = \{a_n\}$ and $b = \{b_n\}$, $|a_n| < 1$ and $|b_n| < 1$ for all n.

3.1. *Question 1*

Give a necessary and sufficient condition on (a, b) for $\mu_a \sim \mu_b$.

Partial answers are:

$$\left.\begin{array}{c} \sum_1^\infty |a_n - b_n|^2 < \infty \\ \sup |a_n| < 1 \end{array}\right\} \Rightarrow \mu_a \sim \mu_b \quad \text{(Peyzière, Brown-Moran)}$$

$$\left.\begin{array}{c} \sum_1^\infty |a_n - b_n|^2 < \infty \\ |a_n| = |b_n| \end{array}\right\} \Rightarrow \mu_a \sim \mu_b$$

(Parreau, Ann. Inst. Fourier 40, 2 (1990), 391–405).

Let us write

$$\mu_{a,\varphi} = \prod_{n=1}^{\infty} \left(1 + \Re(a_n e^{i(\lambda_n x + \varphi_n)})\right)$$

3.2. *Question 2*

$\mu_a \ll \mu_b \Leftrightarrow \mu_{a,\varphi} \ll \mu_{b,\varphi}$.

Fan Ai-Lua is the author of this question. A positive answer would also answer question 1, using the following theorem of Klimer and Saeki (Ann. Inst. Fourier 38, 2 (1988), 63–93) (*cf.* also Fan, Studia Math. (1991) 249–266).

If the φ_n are random with the usual probability,

$$\left.\begin{array}{c} \sum_1^\infty |a_n - b_n|^2 \left(1 + \frac{\cos^2(t_n - s_n)}{\sqrt{2-|a_n-b_n|}}\right) < \infty \\ t_n = \arg(a_n + b_n) \\ s_n = \arg(a_n - b_n) \end{array}\right\} \Leftrightarrow \mu_{a,\varphi} \sim \mu_{b,\varphi} a.s.$$

Motivations and hints can be found in the article of Fan in Bull. Sc. Math. 2^e s., 117 (1993), 421–439.

4. Completeness of sets of complex exponentials in convex sets: open problems

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Let $\Lambda = \{\lambda_n\}$, $n \in \mathbb{N}$, be a sequence of pairwise different complex numbers (points) in the complex plane $\mathbb{C}$, $0 \notin \Lambda$, and $\lambda_n \to \infty$ as $n \to +\infty$.

Let X be a *convex* open or closed set on $\mathbb{C}$. By $H(X)$ denote the space of all continuous complex-valued functions on X which are holomorpic in the interior $\operatorname{Int} X$ of X (if $\operatorname{Int} X \neq \emptyset$) *with the topology of uniform convergence on compact subsets of* X. An exponential system $\operatorname{Exp}\Lambda = \{\exp(\lambda_n z)\}$ is complete in X if the closure of the linear span of $\operatorname{Exp}\Lambda$ in $H(X)$ coincides with $H(X)$.

The completeness problem for a set X is to determine *all* such sequences of exponents Λ for which the system $\operatorname{Exp}\Lambda$ is complete in X. On the background of known results it is natural to look for the solution of the problem in terms of the density of the distribution of the points of Λ and in terms of the geometric characteristics of X. It is natural to subdivide the completeness problem into six cases according to the type of X:
1) $X = [-a, a]$ is a segment on real axis $\mathbb{R}$, $a > 0$, and $H(X) = C[-a, a]$;
2) $X = (-a, a)$, where $a \in (0, +\infty]$, or $X = [0, +\infty)$, or $X = (-\infty, 0]$;
3) $X = G$ is an *unbounded convex* domain in $\mathbb{C}$, $[0, +\infty) \subset G$;
4) $X = \operatorname{Clos} G$, where G is the same as above, $\operatorname{Clos} G$ is the closure of G;
5) $X = G$ is a *bounded convex* domain in $\mathbb{C}$;
6) $X = K$, where K is a *compact convex* set in $\mathbb{C}$, $\operatorname{Int} K \neq \emptyset$;

Below, every item (k-!) or (k-?) is a continuation of item k), and (k-!) (respectively (k-?)) denotes a solved (respectively unsolved) problem.

(1-?) No precise condition is known for the completeness of systems $\operatorname{Exp}\Lambda$ in $[-a,a]$, and finding such a condition is a very difficult problem. In this case we present a test for the completeness of systems $\operatorname{Exp}\Lambda$ in $[-a,a]$ to within a single exponential (see [5, Theorem 7] together with recent results of B. Cole and T. Ransford [2]).

Here and below we denote by $\mathcal{G}$ *the class of all extended Green functions* $g_D(\zeta,0)$ for the point 0 and arbitrary bounded regular (for the Dirichlet problem) domains $D\subset\mathbb{C}$, $0\in D$, $g_D(\zeta,0)\equiv 0$ for $\zeta\notin D$.

THEOREM 1. *If*

$$\sup_{g\in\mathcal{G}}\Big(\sum_n g(\lambda_n)-\frac{a}{\pi}\int_{-\infty}^{+\infty} g(iy)\,dy\Big)$$

equals $+\infty$*, then the system* $\operatorname{Exp}\Lambda$ *is complete in* $[-a,a]$*. Conversely, if this quantity is bounded above, then by deleting a single (arbitrary) exponential from the system* $\operatorname{Exp}\Lambda$ *we obtain a system that is not complete in* $[-a,a]$.

(2-!) In this case the completeness problem was solved completely by the profound Beurling-Malliavin theorem on the radius of completeness [1].
(3-!) When $X=G$ is an unbounded convex domain in $\mathbb{C}$, the completeness problem was solved completely in [3, Theorem 2].
(4-?) The *width* of an unbounded convex domain G, $[0,+\infty)\subset G$, is defined to be the quantity $d_G=\lim_{x\to+\infty} d_G(x)$, where $d_G(x)=\sup\{|z-z'|: z,z'\in G,\ \Re z=\Re z'=x\}$, $x\in[0,+\infty)$.

If either $d_G=+\infty$ or, for all $x\in\mathbb{R}$ we have $d_G(x)\neq d_G<+\infty$, then sharp conditions of completeness of $\operatorname{Exp}\Lambda$ in $\operatorname{Clos}G$ are the same as in (3-!). In the opposite case, there is a test for the completeness of a system $\operatorname{Exp}\Lambda$ in $\operatorname{Clos}G$ only under conditions that the sequence Λ is separated from the imaginary axis (see [4, Corollary 4.2]):

THEOREM 2. *Let* G *be an unbounded convex domain of width* $2\pi d<+\infty$, $[0,+\infty)\subset G$*, and suppose there exists one value of* $x\in\mathbb{R}$ *such that* $d_G(x)=d_G$*. Suppose that a sequence* Λ *satisfies the condition* $|\Re\lambda_n|\geqslant\delta|\lambda_n|$, $n\geqslant n_0$*, for a certain number* $\delta>0$*. The system* $\operatorname{Exp}\Lambda$ *is complete in* $\operatorname{Clos}G$ *if and only if*

$$\sup_{1\leqslant r<R<+\infty}\left(\max\left\{\sum_{\substack{r\leqslant|\lambda_n|<R\\ \Re\lambda_n<0}}-\Re\frac{1}{\lambda_n},\sum_{\substack{r\leqslant|\lambda_n|<R\\ \Re\lambda_n>0}}\Re\frac{1}{\lambda_n}\right\}-d\log\frac{R}{r}\right)=+\infty.$$

(5-?) At present the completeness problem has not been solved satisfactorily for any bounded convex domain G. In our article [5, Theorem 5] we give a complete solution of the completeness problem in a bounded convex domain G in terms of so-called Jensen functions. After [2] this result can be formulated in the following way.

Let G^* be symmetric to G with respect to $\mathbb{R}$, and let $s_G(\theta)$ be the arc length of the boundary of $\operatorname{Clos} G^*$ from a given point to the next (counter-clockwise) point of contact of the supporting line that is orthogonal to the direction θ.

Let $g \in \mathcal{G}$. The function $k_g(\theta) = \int_0^{+\infty} g(te^{i\theta})\,dt$ is called the *indicator of* g. Always the indicator k_g is the support function of a convex compact set K_g such that $0 \in \operatorname{Int} K_g \neq \emptyset$. We set $S(K_g, G) = \frac{1}{2}\int_0^{2\pi} k_g(\theta)\,ds_G(\theta)$. This quantity is the mixed area of the convex sets K_g and G^*.

THEOREM 3. *The system is complete in the convex bounded domain G if and only if* $\inf d \geqslant 1$, *where the infimum is taken over the numbers d for which* $\sup_{g\in\mathcal{G}}\Big(\sum_n g(\lambda_n) - \dfrac{d}{\pi}S(K_g, G)\Big) < +\infty$.

In this theorem, the class $\mathcal{G}$ of Green functions plays the role of test functions. However, the class $\mathcal{G}$ is too wide. Some more transparent sufficient conditions can be extracted from the Theorem 3. For example, they are in [6, Theorem A]. It is possible that these conditions are necessary.

(6-?) No precise condition is known for the completeness of systems $\operatorname{Exp}\Lambda$ in K. The completeness problem in K is apparently a very difficult problem (cf. with $X = [-a, a]$). We present a test for the completeness of systems $\operatorname{Exp}\Lambda$ in K to within two exponentials (see [5, § 7, 3.] together with [2]).

THEOREM 4. *If the quantity* $\sup_{g\in\mathcal{G}}\Big(\sum_n g(\lambda_n) - \dfrac{1}{\pi}S(K_g, K)\Big)$ *equals* $+\infty$, *then the system* $\operatorname{Exp}\Lambda$ *is complete in K. Conversely, if this quantity is bounded above by a finite number, then by deleting two (arbitrary) exponentials from the system* $\operatorname{Exp}\Lambda$ *we obtain a system that is not complete in K.*

References

[1] Arne Beurling and Paul Malliavin *On the closure of characters and the zeros of entire functions.*, Acta Math. 1967. Vol. 118. P. 79–93.

[2] Brian J. Cole and Thomas J. Ransford *Jensen measures and harmonic measures.*, Submitted to Crelle's Journal, June 28, 2000 (to appear).

[3] Bulat N. Khabibullin *On the growth of entire functions of exponential type along the imaginary axis.*, Mat. Sb. 1989. Vol. 180. No. 5. P. 706–719; English transl. in Math. USSR Sb. 1990. Vol. 67. No. 1.

[4] Bulat N. Khabibullin *On the growth of entire functions of exponential type with given zeros along the line.*, Analysis Mathematica. 1991. Vol. 17. No. 3. P. 239–256. (Russian)

[5] Bulat N. Khabibullin *Sets of uniqueness in spaces of entire functions of a single variable.*, Izv. Akad. Nauk. SSSR, Ser. Mat. 1991. Vol. 55. No. 5. P. 1401–1423; English transl. in Math. USSR Izv. 1992. Vol. 39. No. 2.

[6] Bulat N. Khabibullin *Completeness of systems of entire functions in spaces of holomorphic functions.*, Mat. Zametki. 1999. Vol. 66. No. 4. P. 603–616; English transl. in Math. Notes. 1999. Vol. 66. No. 4.

5. Density of Domain of the Weighted Hilbert Transform

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5.1. *Problem 1*

Let Δ be a nonnegative measurable function on the unit circle T. Assume that $\frac{1}{\Delta} \in L^1$ and for definiteness $\|\frac{1}{\Delta}\|_1 = 1$. In this case $f \in L^2(\Delta)$ implies $f \in L^1$, which allows one to define the Hilbert transform Hf for $f \in L^2(\Delta)$:

$$(Hf)(t) = \frac{1}{2\pi i} \oint_T \frac{f(\tau)d\tau}{\tau - t_+} + \frac{1}{2\pi i} \oint_T \frac{f(\tau)d\tau}{\tau - t_-} \ , \ t \in T,$$

where the first and the second integrals are understood as the radial limits from inside and outside of the unit disk D respectively. But Hf need not be in $L^2(\Delta)$. We say that f is in the domain of H on $L^2(\Delta)$ if both f and Hf are in $L^2(\Delta)$. Assume that the domain of H is dense in $L^2(\Delta)$. The question is: can this property be characterized in terms of Δ?

One can show that if $\frac{1}{\Delta} = |g|$, where g is in the Hardy space H^1_+, then the domain of H is dense in $L^2(\Delta)$ if and only if g is an exposed point of the unit ball in the space H^1_+. A point b_0 in a complex or real Banach space B is said to be an exposed point of the unit ball if $\|b_0\| = 1$ and there exists a real continuous linear functional F on B such that $F(b_0) = 1$ and $F(b) < 1$ for all other b in the unit ball. Regarding extreme and exposed points of the unit ball in H^1 see [1], [2], [3] and [4].

Obviously integrability of Δ is a sufficient condition for density of the domain but it is not a necessary one. The interesting case is the one when Δ is not integrable.

5.2. *Problem 2*

Let w be a measurable unimodular function on the unit circle T: $|w(t)| = 1$ for a.a. $t \in T$. Assume that set $P_+ w|H^2_+$ is dense in H^2_+, where H^2_+ is the Hardy space of analytic functions and P_+ is the orthogonal projection from L^2 onto H^2_+. The question is: how this property can be characterized in terms of w?

One can show that the property holds true if and only if w is a canonical solution to a Nehari problem. The Nehari problem consists in finding all the functions w bounded in modulo by 1 on the unit circle T: $|w(t)| \leqslant 1$ for a.a. $t \in T$, with given $P_- w$, where P_- is the orthogonal projection from L^2 onto H^2_-. Details regarding the Nehari problem can be found in [5], [6], [7], [8], [1], [4].

It is also known that w is a canonical solution of a Nehari problem if and only if it is of the form $w = \frac{g}{|g|}$, where g is an exposed point of the unit ball in H^1_+. In this case the representation is unique. See [2], [4] .

References

[1] J. Garnett, *Bounded analytic functions*, Academic Press, (1981)

[2] D. Sarason, *Exposed points in* H^1, Operator Theory: Advances and Applications, Birkhäuser, Part I: Vol. 41, (1989), pp. 485-496; Part II: Vol 48 (1990), pp. 333-347

[3] A. Kheifets, *On regularization of* γ*-generating pairs*, Journal of Funtional Analysis, Vol. 130 (1995), pp. 310-333

[4] A. Kheifets, *Nehari's interpolation problem and exposed points of the unit ball in the Hardy space* H^1, Israel Mathematical conference proceedings, Vol. 11 (1997), pp. 145-151

[5] V.M. Adamjam, D.Z. Arov, M.G. Krein, *Infinite Hankel matrices and generalized problems of Carath éodory-Fejér and M. Riesz*, Funktional. Anal. Appl. 2 (1968), 1-19; English transl.: Funct. Anal. Appl. 2 (1968),1-18

[6] V.M. Adamjam, D.Z. Arov, M.G. Krein, *Infinite Hankel matrices and generalized Carath éodory-Fejér and I. Schur problems*, Funktional. Anal. Appl. 4 (1968), 1-17; English transl.: Funct. Anal. Appl. 2 (1968), 269-281

[7] D.Z. Arov, γ*-generating matrices,* j*-inner matrix-functions and related extrapolation problems*, Teor. Funktii Funktsional. Anal. i Prilozhen. 51 (1989), 61-67; 52 (1989), 57-65; 53 (1990), 57-65; English transl.: J. Soviet Math. 52 (1990), 3487-3491, 52 (1990), 3421-3425, 58 (1992), 532-537

[8] N.K. Nikol'skii, *Treatise on the shift operator*, Grundlehren der mathematishen Wissenshaften 273, Springer, Berlin, 1986 (Translation from Russian edition, Nauka, Moscow, 1980)

6. Harmonic Sliding Analysis Problem

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Harmonic sliding analysis (HSA) is a dynamic spectrum analysis [1] in which the next analysis interval differs from the previous one by including the next signal sample and excluding the first one from the previous analysis interval. Such a harmonic analysis is necessary for time-frequency localization [2] of analysed signals with given peculiarities. Using the well-known Fast Fourier transform (FFT) is not effective in this context. More effective are known recursive algorithms which use only one complex multiplication for computing one harmonic during each analysis interval.

To yield an instant spectrum

$$F_q(p) = \frac{1}{N} \sum_{k=q-N+1}^{q} f(k) W_N^{-pk},\ p \in \overline{0, P-1},\ q = 0, 1, 2, \ \ldots \tag{6.1}$$

it is possible to use a simple recursive algorithm, described in [3], [4]:

$$F_q(p) = F_{q-1}(p) + \frac{1}{N}[f(q) - f(q-N)] W_N^{-pq},\ p \in \overline{0, P-1},\ q = 0, 1, 2, \ \ldots\ . \tag{6.2}$$

This algorithm has a remarkable peculiarity which permits one to organize HSA so that one complex multiplication may be used for computing two, four and even eight (for complex

signals) spectrum harmonics at once [5], [6], [7], [8]. This may be done as follows. Let algorithm (2) be presented as follows:

$$F_q(p) = F_{q-1}(p) + \Delta F_q(p),\ p \in \overline{0, P-1},\ q = 0, 1, 2, \ \dots\ , \tag{6.3}$$

$$\Delta F_q(p) = \frac{1}{N}[f(q) - f(q-N)] \exp[-j\frac{2\pi}{N}pq]. \tag{6.4}$$

The spectrum increments $\Delta F_q(p)$ may be used not only for the spectrum harmonic p, but for spectrum harmonics

$$p_i = iN/4 + p,\ i \in \overline{1, 3} \tag{6.5}$$

and

$$p_k = kN/4 - p,\ k \in \overline{1, 4} \tag{6.6}$$

as well, using known properties of the complex exponential function. In a summarized (and simplified) view the algorithm (3) modification may be presented as follows:
a) for spectrum harmonics (5)

$$F_q(p_i) = F_{q-1}(p_i) + (-j)^{iq}\Delta F_q(p),\ q = 0, 1, 2, \ \dots\ , \tag{6.7}$$

b) for spectrum harmonics (6)

$$F_q(p_k) = F_{q-1}(p_k) + (-j)^{kq}\Delta F_q(-p),\ q = 0, 1, 2, \ \dots\ , \tag{6.8}$$

where $\Delta F_q(-p)$ are complex conjugated spectrum increments $\Delta F_q(p)$, if the signal samples are real, and if the signal samples are complex, $\Delta F_q(-p)$ are generated by inverting the signs of the products of the signal increments $\Delta f_q = \frac{1}{N}[f(q) - f(q-N)]$ with the imaginary part of the weighting function and then forming the appropriate algebraic sums.

In such a way it is possible to use one complex multiplier for computing up to four harmonics for a real signal, and up to eight harmonics for a complex signal, simultaneously.

We can now state the HSA problem: Is it possible to double the speed of the response by using an additional multiplier? If so, how?

References

[1] V.N.Plotnikov, A.V.Belinsky, V.A.Sukhanov and Yu.N.Zhigulevtsev, "Spectrum digital analyzers," Moscow: Radio i svjaz', 1990. - 184 p. (In Russian).

[2] I.Daubechies, "The wavelet transform, time-frequency localization and signal analysis," IEEE Trans.Inform. Theory, vol.36, No.5, pp.961-1005, 1990.

[3] R.D.Lejtes and V.N.Sobolev, "Synthetic telephone systems digital modeling." Moscow: Svjaz', 1969. (In Russian).

[4] J.W.Schmitt and D.L.Starkey, "Continuously updating Fourier coefficients every sampling interval." USA Patent 3778606 Dec.11, 1973.

[5] V.Ya.Krakovsky, "Algorithms for increase of speed of response for digital analyzers of the instant spectrum," Kibernetika, No.5, pp.113-115, 1990. (In Russian).

[6] V.Ya.Krakovskii, "Digital analyzers for dynamic spectral analysis." Meas. Tech. (USA), vol.36, no.12, p.1324-30. Translation of: Izmer.Tekh. (Russia), vol.36, no.12, p.13-16 (Dec.1993).
[7] V.Ya.Krakovskii. "Generalized representation and implementation of speed-improvement algorithms for instantaneous spectrum digital analyzers." Cybernetics and System Analysis, Vol.32, No.4, pp.592-597, March 1997.
[8] V.Ya.Krakovsky. "Spectrum Sliding Analysis Algorithms & Devices." Proceedings of the 1st International Conference on Digital Signal Processing and Its Application, June 30 - July 3, 1998, Moscow, Russia, Volume I, pp.104-107.

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7. Questions on Kazhdan's Property (T) on Hypergroups

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Isolated points of the dual of a locally compact group (endowed with the hull-kernel topology) were first discussed by Diximier [1]. Kazhdan [5] discovered there exists a clear connection between the fact that the class of the one dimensional trivial representation is an isolated point in the dual of a locally compact group (in this case the group is said to have property (T)) and many interesting group properties.

In [6] we have initiated the study of property (T) on hypergroups (with Haar measure), obtaining only some introductory results. We have given an appropriate definition of property (T) for hypergroups: this definition is an extension of the corresponding one for locally compact groups of [3]. Consequently, we say that a hypergroup K has property (T) if each continuous representation of K which has almost invariant vectors has also invariant vectors. (We recall that a representation π of K on the Hilbert space $\mathcal{H}_\pi$ has almost invariant vectors if, for any $\varepsilon > 0$ and $C \subset K$, C compact, there exists $a \in \mathcal{H}_\pi$, with $\|a\| = 1$ such that $\|\pi_x a - a\| < \varepsilon$, $\forall x \in C$; π has invariant vectors if there exists $b \in \mathcal{H}_\pi$, with $\|b\| = 1$, such that $\pi_x b = b, \forall x \in K$.)

We note that in the particular case when K is a locally compact group this definition is equivalent with the one given by Kazhdan [5]. For arbitrary hypergroups, we have only obtained that if K is a hypergroup with property (T), then the class of the one dimensional trivial representation is an isolated point in the dual of K ([6, Theorem 2]), so we ask if the converse is still valid.

It is well known that any amenable non-compact locally compact group has no property (T). This is an immediate consequence of the fact that a locally compact group G is amenable if and only if it satisfies Reiter's condition (P_2): $\forall \varepsilon > 0$, $\forall C \subset G$, C compact, $\exists f \in L_2(G)$, $f \geqslant 0$, $\|f\|_2 = 1$, such that $\|\delta_x * f - f\|_2 < \varepsilon$, $\forall x \in C$, or, equivalently, the left regular representation λ_G of G on $L_2(G)$ has almost invariant vectors; λ_G obviously has no invariant vectors if G is not compact.

For non-compact hypergroups (with Haar measure), the amenability is not equivalent to (P_2). In [7, Example 4.6] an example is given of a non-compact amenable hypergroup that

does not satify (P_2); it is also proved that (P_2) implies the amenability ([7, Theorem 4.1]). Consequently, for hypergroups, we can obtain, with similar arguments as for locally compact groups, that any non-compact hypergroup K satisfying condition (P_2) has no property (T).

For example, if K is a non-compact amenable hypergroup with a supernormal subhypergroup, or if K is a non-compact commutative hypergroup with the Plancherel measure on the dual such that its support contains the trivial character, then K satisfies (P_2) ([7, Theorem 4.7, Lemma 4.5]). In these cases, K has no property (T).

We can not yet give a general answer concerning the relation between amenability and property (T) for the hypergroups case. Thus, we close with the question: Does there exist an amenable non-compact hypergroup having property (T) (?).

References

[1] J. Dixmier, *Points isolés dans le dual d'un groupe localement compact*. Bull. Sc. Math. 85 (1961), 91-96.
[2] J.M.G. Fell, *Weak containment and induced representation of groups.* Canad. J. Math. 14, (1962), 237-268.
[3] P. de la Harpe, A. Valette, *La propriété (T) de Kazhdan pour les groupes localement compacts*. Astérisque 175 (1989).
[4] R. Jewett, *Spaces with an Abstract Convolution of Measures.* Advances in Math. 18 (1975), 1-101.
[5] D. A. Kazhdan, *Connection of the dual space of a group with the structure of its closed subgroups*. Functional Anal. i Prilozen 1 (1967), 71-74.
[6] L. Pavel, *On hypergroups with Kazhdan's property (T).* to appear in Math. Reports.
[7] M. Skantharajah, *Amenable hypergroups.* Illinois J. Math. 36 (1992), 15-46.
[8] M. Voit, *On the dual space of a commutative hypergroups.* Arch. Math. 56 (1991), 380-385.
[9] M. Voit, *Properties of Subhypergroups.* Semigroup Forum 56 (1997), 373–391.
[10] P.S. Wang, *On Isolated Points in the Dual Spaces of Locally Compact Groups.* Math. Ann. 218 (1975), 19-34.

8. Optimal Speech Signal Partition into One-Quasiperiodical Segments

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8.1. *Introduction*

It is well known that analysis of such complicated signals as speech signals has to be carried out synchronically with a current pitch period (quasiperiod). Besides, for speech signal it is important to find current one-quasiperiod segment duration, beginnings and ends as well.

To solve this problem quasi-periodicity and non-periodicity signal models are proposed. Each hypothetical one-quasiperiodical signal segment is considered as a random distortion of previous or following one taken with the unknown multiplying factor. The problem of optimal

current pitch period discrimination and speech signal partition into quasiperiodical and non-periodical segments consists in 1) the finding the best quasiperiod beginnings or the one-quasiperiod segments under restrictions on both value and changing of current quasiperiod duration and multiplying factor and 2) the association of optimal one-quasiperiod segment signals into large quasiperiodic and non-periodic segments. For this problem solving an effective algorithm based on dynamic programming have to be proposed.

8.2. *One-Quasiperiodicity Models*

Let the signal f_n , $n = 1 : N$ be observed where f_n is a signal value at the discrete uniform time $n\Delta t$ with step Δt, for example $\Delta t = 50$ μs for speech signal. If the $(s+1)$-th one-quasiperiod signal segment beginning is denoted by n_s , then $(n_s - 1)$ will be the end of the s-th one-quasiperiod. Further segment signal $f_{n_{s-1}+j}, \quad j = 0 : (T_s - 1)$, $T_s = n_s - n_{s-1}$ will be called s-th one-quasiperiod segment with duration T_s , if it is approximated sufficiently well by neighbouring ones, $(s-1)$-th or $(s+1)$-th, which respectively precedes or follows the s-th one-quasiperiod segment. The latter is taken with the unknown multiplying number α_s^- or α_s^+:

$$f^-_{n_{s-1}+j} = \begin{cases} \alpha_s^- f_{n_{s-2}+j}, & j = 0 : (\min(T_s, T_{s-1}) - 1); \\ 0, & j = \min(T_s, T_{s-1}) : (T_s - 1), \end{cases} \tag{8.1}$$

$$f^+_{n_{s-1}+j} = \begin{cases} \alpha_s^+ f_{n_s+j}, & j = 0 : (\min(T_s, T_{s+1}) - 1); \\ 0, & j = \min(T_s, T_{s+1}) : (T_s - 1). \end{cases} \tag{8.2}$$

Let us introduce a priori restrictions for multiplying number value α and both current quasiperiod duration value T_s and its changing $\Delta_s = T_s - T_{s-1}$:

$$\{\alpha_s : 0 \leqslant \alpha_{\min} \leqslant \alpha_s \leqslant \alpha_{\max}\} = \mathcal{A}, \quad T_{\min} \leqslant T_s \leqslant T_{\max}, \ |\Delta_s| \leqslant \Delta_{\max}. \tag{8.3}$$

Let us fix the elementary quasi-periodicity (EQP) measure for the s-th one-quasiperiodic signal segment $f_{n_{s-1}+j} = f_{n_s - T_s + j}, \quad j = 0 : (T_s - 1)$ as:

$$d\left((n_s, T_s), \Delta_s^-\right) = \min_{\alpha \in \mathcal{A}} \sum_{j=0}^{T_s - 1} \left(f_{n_{s-1}+j} - f^-_{n_{s-1}+j}\right)^2 =$$

$$= \min_{\alpha \in \mathcal{A}} \sum_{j=0}^{\min\left(T_s - \Delta_s^-, T_s\right) - 1} \left(f_{n_s - T_s + j} - \alpha f_{n_s - 2T_s + \Delta_s^- + j}\right)^2 + \sum_{j=\min\left(T_s - \Delta_s^-, T_s\right)}^{T_s - 1} f^2_{n_s - T_s + j} \tag{8.4}$$

or

$$d\left((n_s, T_s), \Delta_s^+\right) = \min_{|\Delta^+| \leqslant \Delta_{\max}} \min_{\alpha \in \mathcal{A}} \sum_{j=0}^{T_s - 1} \left(f_{n_{s-1}+j} - f^+_{n_{s-1}+j}\right)^2 =$$

$$= \min_{0 \leqslant \Delta^+ \leqslant \Delta_{\max}} \left(\begin{array}{c} \min_{\alpha \in \mathcal{A}} \sum_{j=0}^{\min\left(T_s-\Delta^+, T_s\right)-1} \left(f_{n_s-T_s+j} - \alpha f_{n+j}\right)^2 + \\ + \sum_{j=\min(T_s-\Delta^+, T_s)}^{T_s-1} f^2_{n_s-T_s+j} \end{array} \right). \tag{8.5}$$

As it is followed from the expression (8.4-8.5) the signal segment

$$f_{n_{s-1}+j} = f_{n_s-T_s+j}, \quad j = 0 : (T_s - 1)$$

is tested on quasiperiodicity by comparison with previous segment

$$f_{n_s-2T_s+\Delta_s^-+j},\ j = 0 : \left(T_s - \Delta_s^- - 1\right)$$

and all possible following ones $f_{n_s+j},\ j = 0 : (T_s - \Delta^+ - 1)\,,\ |\Delta^+| \leqslant \Delta_{\max}$ but only the best comparison result is associated with the quasiperiodicity measure value $d\left((n_s, T_s)\,, \Delta_s^{\pm}\right)$.

Any permissible variant $\left((n_s, T_s)\,, \Delta_s^{\pm}\right),\ s = 0, 1, 2, ..., P$ of the signal $f_n,\ n = 1 : N$ segmentation on P one-quasiperiodic segments under restrictions (8.3) is characterised by the sum of respective EQP measure values:

$$G\left(n_s,\ s = 0 : P\right) = \sum_{s=0}^{P} d\left((n_s, T_s)\,, \Delta_s^{\pm}\right) \tag{8.6}$$

To find for the signal $f_n,\ n = 1 : N$ the best segmentation onto unknown number P one-quasiperiod segments it is necessary to minimise the criteria (8.6) on all permissible sequences $n_s,\ s = 0 : P$.

8.3. *Problems to be Solved*

The following problems have to be solved.

1. To propose effective dynamic programming algorithm for optimal partition of signal into one-quasiperiodical segments.
2. To determine ways how to unite one-quasiperiodical segments into large quasiperiodic or non-periodic ones.
3. For each time n to formulate some necessary and sufficient conditions that a certain pair $(n^*, T^*)\,,\ n^* < n$ is an optimal one-quasiperiodic segment beginning n^* and duration T^* independently on future signal after n.

References

[1] Taras K. Vintsiuk. Optimal Joint Procedure for Current Pitch Period Discrimination and Speech Signal Partition into Quasi-Periodic and Non-Periodic Segments. - In "Text, Speech, Dialogue", Proc. of the First Workshop on Text, Speech, Dialog - TSD'98, Brno, 1998, pp 135-140.

9. A question of "complexity"

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This problem arises in discrete-time worst-case system identification [9].

In *time-domain* identification we wish to identify the impulse response h of a time-invariant linear system within a prescribed tolerance, using a finite number of sampled values of the output y corresponding to a chosen input signal u. The output signal y is the sum of the system response $u * h$ and a noise term η, so that $y = u * h + \eta$. Both u and h are bounded real or complex valued one-sided sequences, and $*$ denotes the usual convolution. It is assumed that h belongs to some specified model set, such as one of the polynomial sequence sets $\mathcal{P}_n$, or the sets $\mathcal{V}(p, r)$ that are associated with linear systems whose transfer functions H are rational functions and whose poles (if any) occur outside the unit circle. Here H is the z-transform $\widehat{h}$ of the impulse response. In *frequency-domain* identification the aim is to identify H using a finite number of noisy sample values of H on the unit circle. The sample values are obtained by measuring the system's response to a sinusoidal input. It is also assumed that H belongs to some prescribed model set, such as the disc algebra $A(\mathbb{D})$, although additional conditions may be placed on H.

In *worst-case identification* the noise term η is simply assumed to be uniformly bounded and $||\eta||_\infty \leqslant \delta$, where $||\eta||_\infty$ denotes the supremum norm. The ℓ^1, ℓ^2 and H^∞-norms are most often used to measure the accuracy of model estimates (tolerance).

Both time- and frequency-domain worst-case identification problems can be recast within a more abstract framework [7], [2]. Suppose that $\mathcal{X}$ is a normed linear space,

$$\varphi_1, \varphi_2, \ldots, \varphi_N, \ldots$$

a uniformly bounded sequence of continuous linear functionals on $\mathcal{X}$, and that $\tau > 0$. Suppose also that

$$y_k = \varphi_k(h) + \eta_k \text{ and } |\eta_k| \leqslant \delta \text{ for each } 1 \leqslant k \leqslant n,$$

where h is an unknown element of a given subset $\mathcal{M}$ of $\mathcal{X}$. Then, using $y_1, y_2, ..., y_n$, we want to find $\widetilde{h}$ in $\mathcal{M}$ so that $\left\|h - \widetilde{h}\right\| < \tau$. If we can do this, then we say that $\{\varphi_1, \varphi_2, \ldots, \varphi_n\}$ is a (δ, τ)-*identifying set* for $\mathcal{M}$. The connection with time-domain identification is that each $\varphi_k(h) = (u * h)_k$, where u is the chosen input, while for frequency-domain identification $\varphi_k(h) = H(z_k) = \widehat{h}(z_k)$ where $z_0, z_1, ..., z_{n-1}$ are points on the unit circle.

The *complexity* of identification in $\mathcal{M}$ for a given tolerance τ and noise bound δ is defined to be the minimum number of 'observations' or functionals required to obtain an estimate within that tolerance for the given noise bound. It depends on $\mathcal{M}$ and on the type of functionals that are allowed. Since $\|f\|_2 = \|f\|_{H^2} \leqslant \|f\|_{H^\infty} \leqslant \|f\|_1$ for any sequence f, the complexity of identification in $\mathcal{M}$ decreases as we replace the ℓ^1 norm on $\mathcal{M}$, by the H^∞ norm, and then by the ℓ^2 norm. It is known that ℓ^1 identification is typically 'exponential' in

complexity, and so not very practical (see [1], for example). On the other hand, both H^∞ and ℓ^2 identification are typically 'polynomial' [3], [5], [8].

A drawback to using the conservative ℓ^∞ norm to measure the noise component is that a single outlier may make this very large, and this in turn may make it difficult to 'identify' the system using standard techniques. An obvious way to address this difficulty is to replace the ℓ^∞ norm by a norm that is less sensitive to outliers. More generally we work with a sequence $(\|\|\|_n)$ of seminorms on $\mathbf{R}^n$, assuming that each is dominated by the ℓ^∞ norm. The problem then is to determine the complexity for different choices of $\mathcal{M}$ and norms on the noise.

We are helped in this task by the observation [3], [2], [7], that when the ℓ^∞ norm is used to measure the noise, then linear functionals $\varphi_1, \varphi_2, \varphi_3, \ldots, \varphi_n$ form a (δ, τ)-identifying set for an absolutely convex set $\mathcal{M}$ if and only if

$$\max_{1 \leqslant k \leqslant n} |\varphi_k(h)| \geqslant \delta \text{ for each } h \in \mathcal{M}_\tau,$$

where $\mathcal{M}_\tau = \{h \in \mathcal{M} : \|h\| = \tau\}$.

A related result [6] for the generalised noise measure case is that there is a 'robustly convergent' algorithm for estimating h on the basis of n test functional values if and only if there is a number $\varepsilon > 0$ such that

$$\liminf_{n \to \infty} \|(\varphi_1(h), \varphi_2(h), ..., \varphi_n(h))\|_n \geqslant \varepsilon \|h\| \text{ for each } h.$$

This is relevant because it can be shown that if there is such an algorithm then for any noise bound δ and tolerance level τ there is a finite subset of the φ_ks that form a (δ, τ)-identifying set for $\mathcal{M}$.

For a concrete version of the problem, what is the complexity of identification if we suppose that $\mathcal{M} = A(\mathbb{D})$ with its usual norm, and that $\|\|\|_n = \|\|\|_*$ for all n, where $\|\|\|_*$ is an *Orlicz* or *Lorenz* norm on $A(\mathbb{D})$? Of particular interest is the case of the Lorenz norm given by $\|\mathbf{x}\|^w = \|\mathbf{x}\|_w / \|(1, 1, ..., 1)\|_w$, where

$$\|\mathbf{x}\|_w = \sup_{\pi \in \Sigma_n} \sum_{j=1}^{n} \left|x_{\pi(j)}\right| w_j \text{ for each } \mathbf{x} = (x_1, x_2, ..., x_n) \in \mathbf{R}^n,$$

and Σ_n denotes the set of permutations of $\{1, 2, ..., n\}$, and where $\mathbf{w} = (1, 1, ..., 1, 0, 0, .., 0)$, with the first K terms equal to 1.

References

[1] M.A. Dahleh, T. Theodosopoulos and J.N. Tsitsiklis, The sample complexity of worst-case identification of FIR linear systems, *Systems Control Lett.*, **20** (1993), 157-166.

[2] D.W.Hadwin, K.J.Harrison and J.A.Ward, Worst-case identification of linear systems: existence and complexity, in *Proc. Centre for Math. and its Applications*, **36** (1999), 53-65.

[3] Harrison, K.J., J.R. Partington and J.A. Ward, Complexity of identification of linear systems with rational transfer functions, *Math. Control Signals Systems*, (1998)

[4] Harrison, K.J. and J.A. Ward, Fractional covers for convolution products, *Result. Math.*, **30** (1996), 67-78.

[5] Harrison, K.J., J.A. Ward and D.K. Gamble, Sample complexity of worst-case H^∞-identification, *Systems Control Lett.*, **27** (1996), 255-260.
[6] Makila, P.M. and J.R. Partington, Robustness in H^∞ identification, preprint 1999.
[7] Partington, J.R., Interpolation in normed spaces from values of linear functionals, *Bull. London Math. Soc.*, **26** (1994), 165-170.
[8] Partington, J.R., Worst-case identification in ℓ^2: linear and non-linear algorithms, *Systems Control Lett.*, **22** (1994), 93-98.
[9] Partington, J.R., *Interpolation, identification and sampling*, Oxford University Press, 1997.

10. Rate of decay of convolution vs. frequency of sign changes

H.S. Shapiro

All references, as well as further background discussion concerning the present problem may be found in reference [S].

Let f be in $L^\infty(\mathbb{R}^+)$ (the class of real-valued bounded measurable functions on $(0,\infty)$). Then, the following, due to B.F. Logan, Jr., is known: If

$$F(y) := \frac{2}{\pi}\int_0^\infty \left(\frac{y}{x^2+y^2}\right) f(x)\,dx, \quad y>0 \tag{10.1}$$

satisfies

$$F(y) = O(e^{-ay}) \quad \text{as } y\to\infty \tag{10.2}$$

for some $a>0$, then $\tilde{f}$, *the even extension of* f *to* $\mathbb{R}$ (which is in $L^\infty(\mathbb{R})$) *has spectrum disjoint from* $(-a,a)$. the converse is also true. (The *spectrum* here means the support of the distributional Fourier transform.) As an illustration, look at $f(x)=\cos ax$ (then, $\tilde{f}(x)=\cos ax$, $x\in\mathbb{R}$). Here $F(y)$ is the Poisson integral of $\cos ax$, evaluated at a point of the imaginary axis, so $F(y)=e^{-ay}\cos ax$. Observe that in this case, $f(x)$ *has an essential sign change on each interval in* $\mathbb{R}^+$ *of length greater than* π/a (that is, on each such interval it assumes positive values, as well as negative values, on a set of positive measure). In a 1965 doctoral thesis, B.F. Logan, Jr. raised the question whether (10.1) implies an asymptotic lower bound for the amount of oscillation of f. Namely, defining $\sigma(x)$ as the number (possibly infinite) of points of $(0,x)$, on each neighborhood of which f has an essential sign change, he asked whether

$$\liminf_{x\to\infty} \frac{\sigma(x)}{x} \geqslant \frac{a}{\pi}, \tag{10.3}$$

For each $f\in L^\infty(\mathbb{R})$, not identically zero and satisfying (10.2). He proved the answer is affirmative if f also is assumed to *be the restriction to* $\mathbb{R}^+$ *of an entire function of exponential type*. So far as I know, no one has proved (or disproved) this assertion without that last hypothesis.

In my paper [S] I remarked that, as a consequence of a recent theorem due to Baouendi and Rothschild, the weakening of (10.2) to

$$F(y) = O(y^{-n}), \quad y \to \infty \tag{10.4}$$

for every positive integer n implies the (weak) oscillation result: f *has an essential sign change on* (b, ∞) for every $b > 0$.

Certain questions now almost pose themselves: Suppose $F(y)$ has, as $y \to \infty$, a rate of decrease intermediate between (10.2) and (10.4) (e.g., $F(y) = O(e^{-y^t})$ for some t with $0 < t < 1$.) Can one assert anything about the frequency of sign changes of f, beyond what already follows from (10.4)?

A further avenue of generalizations appears when we observe that (10.1) is a convolution on the group $\mathbb{R}^+$ (with respect to the Haar measure $\frac{dx}{x}$). After a logarithmic variable change it becomes a usual convolution on $\mathbb{R}$, with the "kernel" $K(x) := (2/\pi)(\cos x)^{-1}$ (details in [S]). Thus, all the questions we have raised so far can be put in the form: Deduce from the rate of decay at $+\infty$ of $g \star K$, for some $g \in L^\infty(\mathbb{R})$, lower bounds for the (asymptotic frequency of) essential sign changes of g. Once this standpoint is taken, one can raise these questions for other kernels, like $K(x) = e^{-x^2}$.

One final remark: It is a corollary of the result that (10.2) implies disjointness of spectrum $\tilde{f}$ from $(-a, a)$, that: *If (10.2) holds for every* $a > 0$, *then* f *vanishes a.e.* This result predates Logan's work, and is a special case (after transformation from $\mathbb{R}^+$ to $\mathbb{R}$ by the logarithmic variable change) of general results due to I.I. Hirschmann, Jr. from 1951. We might express matters thusly: for some class of kernels in $L^1(\mathbb{R})$, Hirschmann found the *critical* rate at which a convolution of a nontrivial function in $L^\infty(\mathbb{R})$ with this kernel may decay at ∞ (i.e., faster decay is impossible). There is some evidence that *substantial* decay implies corresponding oscillatory behavior; this seems a promising and mostly unexplored area.

References

[S] Shapiro, H.S., *Notes on a theorem of Baouendi and Rothschild*, Expositions Math. **13** (1995) 247–275.

[G. Tsoucari, K. Bethanis, P. Tzamalis, and A. Hountas] G. Tsoucari,[1] K. Bethanis,[2] P. Tzamalis,[2] and A. Hountas[2]

[Direct Methods and Quantum Mechanics] Direct Methods and Quantum Mechanics

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11. The Problem

Direct Methods for crystal structure determination are based on mathematical relations, so called *phase relations*, between the moduli (observed by diffraction experiments) and the (unknown) phases of the Fourier coefficients E(H) of the periodic electron density ρ(r). The latter can be approximated by one electron quantum mechanical *wave functions* ψ*(r)*:

(11.1) $$\rho(r) = |\quad \psi(r)^2| \Leftarrow FT \Rightarrow E(p) = \Psi(p) * \Psi(-p)^*$$
$$\psi \quad \Leftarrow FT \Rightarrow \quad \Psi$$

A question arises then, whether it is possible to obtain *phase relations from fundamental Quantum Mechanics.* We show below that the Schrodinger equation in Fourier (momentum) space, written below in appropriate atomic units, provides a basis for such relations:

Direct space Momentum space

(11.2) $$-\Delta\psi(r)/2 + V(r)\psi(r) = \varepsilon_0\psi(r) \Leftarrow FT \Rightarrow p^2\Psi(p)/2 + W(p) * \Psi(p) = \varepsilon_0\Psi(p)$$

with V $\Leftarrow$ FT $\Rightarrow$ W

For a periodic crystalline structure the convolution integral in momentum space is replaced by a discrete summation and eq. (2) is re-arranged as (3). We see then (with an eigenvalue $\varepsilon_0 < 0$) *that the phase of the wave function Ψ(p) is invariant under the potential (convolution) operator W(p)*$*$:

(11.3) $$(H^2/2 - \varepsilon_0)\Psi(H) = -\Sigma_K W(K) \quad \Psi(H - K)$$

The next key remark is that the Fourier Coefficients W(K) of the potential function V(r) are identical to the crystallographic expression - Z $\sqrt{}$N E(K) / K^2. For a unit cell containing N identical atoms of atomic number Z we have, as shown in Appendix:

(11.4) $$W(K) = -Z\sqrt{N}E(K)/K^2$$

Eq. (4) is the *key relation* linking the Quantum Mechanical potential function to the diffraction experiment for a crystal. Thus eq. (3) is written as (5), as shown in Appendix

(11.5) $$(H^2/2 - \varepsilon_0)\Psi(H) = Z\sqrt{N}\Sigma_K E(K)\Psi(H - K)/K^2$$

(11.6) $$E(H) = \Sigma_K \Psi(K)\Psi^*(K - H)$$

The pair of eq. (5) and (6) forms a system of self consistent equations, that is a usual procedure in Quantum Mechanics. They provide the physical basis of the TWIN algorithm developed for crystal structure determination (Hountas, A. and Tsoucaris, G. (1995) Acta Cryst. A51, 754-763; see also: J. Navaza and G. Tsoucaris, in Phys. Rev. (1981); G. Berthier et al. in J. Quantum Chemistry, 1996, p. 195-199). The final form (5) of the Schrodinger equation in momentum space has a strong similarity with one of the fundamental phase relations of Direct Methods:

(11.7) $$Phase \quad of \quad E(H) = Phase \quad of \quad [\Sigma_K E(K)E(H - K)]$$

Note that the positive factor $1/K^2$ in eq. (5) plays the role of a weighting factor for each contributor E(K) Ψ(H-K) in the summation, that is a usual technique in Direct Methods.

The similarity becomes closer with a further approximation related to the classical Linear Combination of Atomic Orbitals LCAO method:
Ψ(H) = c E(H) with a known constant $c > 0$.

In conclusion, we have shown a close relation between a fundamental formula in Direct Methods (obtained by Probability theory applied to the FT of the electron density of a crystal) and the Schrodinger equation in momentum (i.e. FT) space. We further note that the FT between position and momentum is a central notion in Quantum Mechanics. It corresponds to a kind of "built in" feature of Quantum Mechanics and constitutes the fundamental link between the position and the momentum of a quantum mechanical particle, well known as the Uncertainty Principle.

Note: The above presentation holds for a simplified model of electrons moving independently to each other (no interelectronic interaction) in the potential created by the nuclei of the crystal. Such an approximation is of course inappropriate for a correct quantum description of molecular orbitals, but it is sufficient for the determination by Direct Methods of approximate phases of the Fourier coefficients EH (with observed moduli).

12. Appendix

The electron-nuclei attractive potential for N atoms of atomic number Z_j at positions r_j is (in atomic units):

$V(r) = - \Sigma j \; Z_j \; / \; |r - r_j|$ with $r \in R^3$

If r plays the role of time and $K \in R^3$ that of frequency, then the FT at K of V(r) is :

$W_K = - \Sigma_j \; [\; Z_j \; \exp (\; 2\pi \; i \; K. \; r_j \;) \;] \; / \; K^2$

reminding that in 3D we have:

$1/|r| \quad \Leftarrow FT \Rightarrow 1/|K|^2$

Note that for simplicity the above notation of modulus for the 3D vectors r and K has been omitted throughout the text.

The Fourier coefficients E_K (so called normalized structure factors) involved in diffraction experiments have a similar expression apart for the (positive) factor $1/K^2$. Indeed, the FT at K of N identical atoms -considered as Dirac masses $1/\sqrt{N}$ at positions r_j - is given by:

$E_K = \Sigma j \; [\; \exp (\; 2\pi \; i \; K. \; r_j \;) \;] \; / \; \sqrt{N}$

For atoms of atomic number Z, eq. (4) follows.