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CONSISTENCY AND SYMMETRY CONDITIONS FOR LINE PROJECTIONS

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We present some relations between experimental spectra representing line projections of electronic densities in the momentum space. All spectra which are the projections of the same density, must be interdependent. It can be derived from the consistency condition and symmetry of the line projections. The knowledge of these dependences, found in the paper, can be utilised for an improvement of experimental data as e.g. two-dimensional angular correlation of positron annihilation spectra.

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1. Introduction

The *consistency condition* (CC) has been considered in different manner by many authors [1–3] for reconstructing densities $\rho(\boldsymbol{p})$ from their line projections. Mathematically it is stated by the CC of Helgason–Ludwig [4, 5], shortly described in the next section. This condition is satisfied if each of the projections is complete, i.e. if it is measured up to such a momentum $p_{\max}$ above which $\rho(\boldsymbol{p})$ is isotropic and all projections have the same values. On the contrary to some medical investigations, this restriction is usually satisfied in the case of measurements of two-dimensional angular correlation of positron radiation (2D ACAR) spectra. Of course, for a proper reconstruction of $\rho(\boldsymbol{p})$, the densities above $p_{\max}$ should have negligible values (e.g. [6]).

The CC, automatically imposed on the data via reconstruction, can also be utilised for an improvement of those experimental data for which $\rho(\boldsymbol{p})$ is not reconstructed, as well as for checking (before the reconstruction) if they were measured (and next corrected in order to remove various experimental imperfections) properly. For that reason it is necessary to expand the data into some orthogonal polynomials series. We propose the Chebyshev polynomials which are unique because they are the only polynomials with zeros known analytically. It allows to apply (in calculating of the expansion coefficients c_m) the Gaussian quadrature formulae in a very simple way (last expression in Sec. 2.2).

In this paper we present some relations between c_m derived from both the CC and a symmetry of $\rho(\boldsymbol{p})$. A fulfilment of these relations is illustrated on an example of some model projections. A way of choosing $p_{\max}$ is discussed in the last section.

2. Theory

In the case of reconstructing $\rho(\boldsymbol{p})$ from the line projections $N(p_x, p_y)$ (on a chosen plane $p_y = \text{const}$), both functions are described in the polar system where $N(p_x, p_y) \equiv N(t, \varphi)$ and $\rho(p_x, p_z) \equiv \rho(p, \theta)$. Here $t = |p_x|/p_{\max}$ and φ denote a distance of the integration line from the origin of the coordinate system and its angle with respect to a chosen axis of an investigated object, respectively. In this way all projections measured in the Cartesian coordinates connected to the apparatus are described in the same coordinate system (in our case in such a reciprocal lattice system where a symmetry of $\rho(\boldsymbol{p})$ is described).

2.1. Consistency condition of Helgason–Ludwig

For two-variable function $N(t, \varphi)$, defined over the complete domain $\Gamma = \{(t, \varphi), -1 \leq t \leq 1, 0 \leq \varphi \leq 2\pi\}$ and being a projection of $\rho(p, \theta)$ supported on the unit disk, the following three conditions are necessary and sufficient:

1°. Picard condition: the norm of $\rho(p, \theta)$ must be finite.

2°. Projection-moment theory condition: $a_{kn} = 0$ for $|l| > k$.

3°. Symmetry condition: $a_{kn} = 0$ for $|l| + k$ *odd*.

a_{kn} denotes a coefficient of the expansion into the Fourier series of $a_k(\varphi)$, where $a_k(\varphi)$ is the k-th moment of the projection $N(t, \varphi)$ with respect to the variable t

$$a_k(\varphi) = \int_{-1}^{1} N(t, \varphi) t^k \mathrm{d}t, \tag{1}$$

where k is a nonnegative integer. After expanding $a_k(\varphi)$ into the Fourier series

$$a_k(\varphi) = \sum_{-\infty}^{\infty} a_{kn} \exp(\mathrm{i}n\varphi), \tag{2}$$

the Fourier coefficients a_{kn} are as follows:

$$a_{kn} = \frac{1}{2\pi} \int_0^{2\pi} a_k(\varphi) \exp(-\mathrm{i}n\varphi) \mathrm{d}\varphi. \tag{3}$$

The fact that the projections are periodic with respect to φ, i.e. $N(t, \varphi)$ and $N(t, \varphi + \pi)$ represent integrals of $\rho(\boldsymbol{p})$ over the same line, leads to the condition 3°.

2.2. Cormack's method with symmetry conditions

In the Cormack method [1] both functions $\rho(p, \theta)$ and $N(t, \varphi)$ are expanded into the polar Fourier series. According to [7], the most suitable way of reconstructing $\rho(\boldsymbol{p})$ is to perform reconstruction on the planes $p_y = \text{const}$, perpendicular to the main axis of the crystal rotation where the number of equivalent directions is maximal. Then all series reduce to the cosine series

$$\rho(p) = \sum_{n=0}^{\infty} \rho_n(p) \cos(n\Theta), \tag{4}$$

$$N(t, \varphi) = \sum_{n=0}^{\infty} N_n(t) \cos(n\varphi), \tag{5}$$

with $n = 0 \bmod |G|$ where $|G|$ denotes the order of the main rotation axis ($n = 0$, 4, 8,...etc. or $n = 0$, 6, 12,...etc. for cubic and tetragonal or hexagonal structures,

respectively). If N_n is expanded into a series of the Chebyshev polynomials of the second kind (U_k):

$$N_n(t) = 2\sum_{m=0}^{\infty} a_n^m \sqrt{1-t^2}U_{n+2m}(t), \tag{6}$$

then $\rho_n(p)$ is described by a series of Zernike polynomials where a_n^m can be derived from the orthogonality relation for $U_k(t)$:

$$a_n^m = \frac{2}{\pi}\int_0^1 N_n(t)U_{n+2m}(t)\mathrm{d}t. \tag{7}$$

The last equation is given in the unit system where $p_{\max} \equiv 1$ (above $p_{\max}$ the density is equal to zero). Choosing $t = \cos\psi$, Eq. (6) becomes

$$N_n(t) = 2\sum_{m=0}^{\infty} a_n^m \sin[(n+2m+1)\psi], \tag{8}$$

which is equivalent to the expansion of $N_n(t)$ into a series

$$N_n(t) = 2\sum_{m=0}^{\infty} \tilde{a}_n^m \sin[(2m+1)\psi], \tag{9}$$

where the first $n/2$ coefficients $\tilde{a}_n^m$ are equal to zero. It is the CC being equivalent to the requirements 2° and 3° (here only even polynomials are used) — see Sec. 2.1. In the unit system $t = \cos\psi$, Eq. (7), written below for $\tilde{a}_n^m$, becomes

$$\tilde{a}_n^m = \frac{1}{M}\left[\sum_{j=1}^{M-1} N_n(\cos[j\Delta_\psi])\sin([2m+1]j\Delta_\psi) + \frac{1}{2}(-1)^m N_n(0)\right],$$

where ψ is equidistant with some step $\Delta_\psi = 2\pi/M$. M denotes a number of points used in evaluating of a (in this way the Gaussian quadrature formulae are applied).

3. Consistency conditions for symmetry objects

Let us write Eq. (5) for such cases when three and four projections are measured (on the plane $p_y = \text{const}$, perpendicular to the rotation axis of the order $|G|$) with φ changed (at equal steps) from zero up to $\varphi_G = \pi/|G|$. Then, the radial functions $N_n(t)$ are described by the following sets of the equations:

$$N_0(t) = (1/4)[N(t,0) + 2N(t,\varphi_G/2) + N(t,\varphi_G)],$$

$$N_{|G|}(t) = (1/2)[N(t,0) - N(t,\varphi_G)],$$

$$N_{2|G|}(t) = (1/4)[N(t,0) - 2N(t,\varphi_G/2) + N(t,\varphi_G)]$$

for $K = 3$ while for $K = 4$ we have

$$N_0(t) = (1/6)[N(t,0) + 2N(t,\varphi_{|G|}/3) + 2N(t,2\varphi_{|G|}/3) + N(t,\varphi_{|G|})],$$

$$N_{|G|}(t) = (1/3)[N(t,0) + N(t,\varphi_{|G|}/3) - N(t,2\varphi_{|G|}/3) - N(t,\varphi_{|G|})],$$

$$N_{2|G|}(t) = (1/3)[N(t,0) - N(t,\varphi_{|G|}/3) - N(t,2\varphi_{|G|}/3) + N(t,\varphi_{|G|})],$$

$$N_{3|G|}(t) = (1/6)[N(t,0) - 2N(t,\varphi_{|G|}/3) + 2N(t,2\varphi_{|G|}/3) - N(t,\varphi_{|G|})].$$

Now we expand the measured projections into the Chebyshev polynomial series

$$N(t,\varphi) = 2\sum_{0}^{\infty} c_m(\varphi)\sin([2m+1]\psi). \tag{10}$$

Introducing Eqs. (9) and (10) into the above sets of the equations for $N_n(t)$, we get the same two sets of the equations but for $\tilde{a}_n^m$ and $c_m(\varphi)$. For example, for $K = 3$ and $n = 0$ we have

$$\tilde{a}_0^m = [c_m(0) + 2c_m(\varphi_G/2) + c_m(\varphi_G)]/4.$$

Knowing that the first $n/2$ coefficients $\tilde{a}_n^m$ are equal to zero for each n, the following dependence between $c_m(\varphi)$ is obtained:

1. $|G|/2$ first coefficients $c_m(\varphi)$ (c_0, c_1, c_2 or c_0, c_1 for cubic or hexagonal structure, respectively) are the same for all projections, i.e. $c_m(\varphi) = c_m = \tilde{a}_0^m$.
2. $|G|$ first coefficients $c_m(\varphi)$ satisfy a dependence: $2c_m(\varphi_G/2) = c_m(\varphi) + c_m(\varphi_G - \varphi)$.

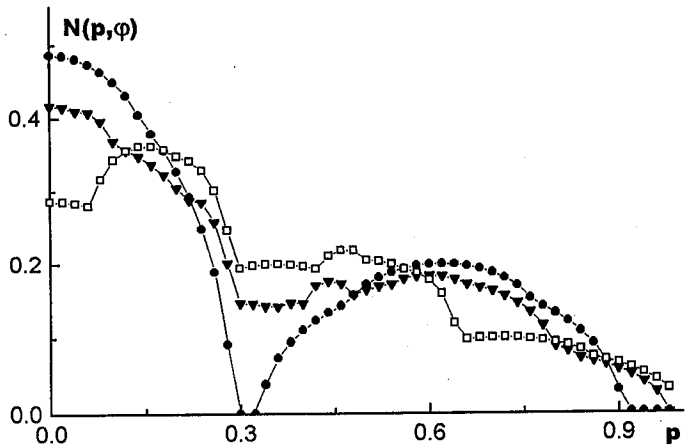

Fig. 1. Line projections of $\rho(p)$ having hexagonal symmetry for $\varphi = 0$ (circle), $\varphi = \varphi_G/2 = \pi/12$ (triangle) and $\varphi = \varphi_G = \pi/6$ (square) with φ changed on the plane perpendicular to the hexagonal axis.

All these conditions have been proved for various models of $\rho(p)$. In Fig. 1 three projections of a strongly anisotropic model density, having symmetry $|G| = 6$ ($\varphi_G = \pi/6$), are displayed. In spite of their quite different shape, three first $c_m(\varphi)$ are the same for all $N(t,\varphi)$ being independent of φ and the next $c_m(\varphi)$ satisfy the relation 2.

4. Conclusions

All spectra received from experiment are contaminated by statistical noise and because of that they are not consistent. Depending on a number of measured projections, some part of the inconsistent noise is eliminated via the consistency

conditions during the reconstruction of $\rho(\boldsymbol{p})$. However, we propose to check (before the reconstruction) if the inconsistent part of the data is not too large [8]. In this way we learn if the spectra were measured and next corrected properly. For this purpose we can use some interdependences, derived by combining the consistency and the symmetry conditions, obtained here for the line projections. Of course, they can also be utilised for an improvement of such data for which the density is not reconstructed.

All relations derived in the paper are valid for any $p_{\max}$ so long as $p_{\max} \geq p_{\mathrm{a}}$, where p_{a} denotes the momentum above which $\rho(\boldsymbol{p})$ is isotropic. In the case of 2D ACAR spectra above p_{a} we should have only the isotropic core contribution. Of course, the value of p_{a} depends on an investigated material — see the book [8] where the electron densities $\rho(\boldsymbol{p})$ are presented for almost all elemental solids. For example, for iridium $p_{\mathrm{a}} = 3$ [a.u.] (atomic unit) while for strontium $p_{\mathrm{a}} = 1.5$ [a.u.]. Taking into account the effect of the positron wave function and the electron–positron (e–p) correlation effects, in the case of the e–p densities one can expect the value of p_{a} lower than 3 a.u.

In the case of reconstructing $\rho(\boldsymbol{p})$, in the above definition of $p_{\max}$, p_{a} should be replaced by p_0. Here p_0 denotes the momentum above which the core contribution (in comparison with values of the total densities $\rho(\boldsymbol{p})$ for lower momenta) is negligible. In order to choose p_0 properly, we recommend results of the paper [9] where $\rho^{\mathrm{core}}(p)$ for the e–p momentum densities was calculated within the local density approach. According to our experience (being in agreement with the results of the paper [9]) a choice of $p_{\max}$ of the order 3 [a.u.] (usually 2D ACAR spectra are measured up to 3 [a.u.] with number of counts about 1000 times lower than at peak) is quite sufficient.

Acknowledgments

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References

[1] A.M. Cormack, *J. Appl. Phys.* **34**, 2722 (1963); **35**, 2908 (1964).

[2] (a) R.M. Lewitt, *Proc. IEEE* **71**, 390 (1983); (b) R.M. Lewitt, R.H.T. Bates, *Optik* **50**, 189 (1978).

[3] H. Kudo, T. Saito, *J. Opt. Soc. Am. A* **8**, 1148 (1991).

[4] S. Helgason, *Acta Math.* **113**, 153 (1965).

[5] D. Ludwig, *Commun. Pure Appl. Math.* **19**, 49 (1966).

[6] R.M. Lewitt, R.H.T. Bates, *Optik* **50**, 19 (1978).

[7] G. Kontrym-Sznajd, *Phys. Status Solidi A* **117**, 227 (1990).

[8] N.I. Papanicolaou, N.C. Bacalis, D.A. Papaconstantopoulos, *Handbook of Calculated Electron Momentum Distributions, Compton Profiles and X-Ray Factor of Elemental Solids*, CRC Press, Florida 1991.

[9] S. Daniuk, M. Šob, A. Rubaszek, *Phys. Rev. B* **43**, 2580 (1991).