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THE PSEUDOINVERSE MATRIX AND THE METHODS OF BAND CALCULATION

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The basic equation of the augmented plane waves method was derived in the spherical harmonics representation. It is possible to subdivide the structural and the potential parts of this equation. A new form of the Kohn–Korringa–Rostoker-equation with the analogous properties was received.

1. INTRODUCTION

THE MAIN tool used in the present work is a pseudoinverse matrix. In detail its theory is outlined, e.g. in [1]. All the required information is given briefly in the Appendix. Here we will formulate only several key aspects necessary for the understanding of this paper's main text.

The pseudoinverse matrix is called a matrix inverse to a degenerated matrix, i.e. to that which transforms some subspace of a space under transformation into zero. A classic example of a degenerated matrix is a rectangular matrix having a number of rows p less than a number of columns n. If the matrix rank equals p (it means that its rows, considered as n-dimensional vectors, are linearly independent), a space R^n is transformed by the matrix into a space R^p and, consequently, some subspace of n–p dimension is transformed into zero. This subspace is referred to as a kernel of a matrix A, Ker A. In the Appendix it shown that Ker A coincides with the orthogonal complementation to the subspace span on p row-vectors of the matrix A. The latter subspace is called the carrier of the matrix A, Car A. No vectors of Car A are transformed into zero by the matrix A, i.e. the matrix A realizes a one-valued transformation of Car A onto R^p. In this case it is clear that a transformation inverse to A is defined naturally as a transformation acting from R^p to Car A. In the Appendix it is shown the way to build such a matrix. We will denote it A^{-1}, in order to stress that a pseudoinverse matrix – when operated carefully – is the true object of the matrix theory the same as an ordinary inverse matrix. Let us outline some pseudoinverse matrix properties which will be used in what follows.

1. For rectangular matrices appearing in band calculation n is the number or plane waves used (or augmented plane waves), while $p = l_{\max}^2$, where $l_{\max} - 1$ is the maximal value of azimuth quantum number l. Typically in band calculations $p < n$ or even $p \ll n$ and p rows of the matrix A are linearly independent.

2. If A and B are rectangular matrices, A^{-1} and B^{-1} pseudoinverse matrices, then

$$(A^{-1})^* = (A^*)^{-1}, \quad (AB)^{-1} = B^{-1}A^{-1},$$

where, as always, A^* is the matrix transposed and complex conjugated with respect to the matrix A.

3. Vectors of a space R^n of a greater dimension will be designated by symbols $\mathbf{u}, \mathbf{t}, \ldots$ while vectors of a space R^p of a lesser dimension by symbols $\mathbf{f}, \mathbf{g}, \ldots$. In this case, if $\mathbf{u} \in$ Car A, then $A\mathbf{u} = \mathbf{f} \neq \mathbf{0}$ and $\mathbf{u} = A^{-1}\mathbf{f}$; if, however, a vector $\mathbf{u}$ does not belong to the matrix A carrier, such vector cannot be represented in the form $A^{-1}\mathbf{f}$.

In Section 2 the basic equation of the augmented plane waves (APW) [2] is reformulated from the representation of quasiwave vectors (k-representation) into the representation of spherical harmonics (l-representation). The possible consequences of a reformulation are discussed. In Section 4 the KKR-method [3] of band calculations is analyzed analogously. The main result here is the new form of the basic equation of the KKR-method in l-representation.

2. THE APW-METHOD

In the frame of the APW-method the main problem is to find a value of parametric energy E, that satisfies the equation

$$\det |M_{ij} + F_{ij}(E) - EJ_{ij}| = 0, \tag{1}$$

where

$$J_{ij} = \delta_{ij}\Omega_0 - 4\pi R^2 \frac{j_1(k_{ij}R)}{k_{ij}}, \tag{2}$$

Ω_0 is a unit cell volume, R is MT-sphere radius, $j_1(x)$

is the spherical Bessel function; $k_{ij} = |\mathbf{k}_{ij}| = |\mathbf{k}_i - \mathbf{k}_j|$, $\mathbf{k}_i = \mathbf{k} + \mathbf{K}_i$, where $\mathbf{k}$ is the reduced wavevector and $\mathbf{K}_i$ are reciprocal lattice vectors which distinguish the augmented plane waves (APW's); i, j run from 1 to n. Then

$$M_{ij} = (\mathbf{k}_i, \mathbf{k}_j)J_{ij}, \tag{3}$$

$$F_{ij}(E) = 4\pi R^2 \sum_{l=0} (2l + 1) \times P_l(i, j) j_l(k_i R) j_l(k_j R) L(u_l), \tag{4}$$

where $P_l(i,j)$ is the Legendre polynomial of the cosine of the angle between $\mathbf{k}_i$ and $\mathbf{k}_j$,

$$L(u_l) = \frac{u_l'(R, E)}{u_l(R, E)}, \tag{5}$$

is the value of the logarithmic derivative of the solution $u_l(r, E)$ of the radial Schrödinger equation for $r = R$; u_l and $L(u_l)$ depend on the parametric energy E and the crystal potential.

If E satisfies the determinant equation (1), then it is eigenenergy of the system. To determine all eigenenergies, it is necessary to obtain all the solutions of equation (1) varying E over the examined energy interval.

It is known, that for every atom in unit cell one has to account 30–50 APW's. For instance, the calculation of a two-atomic compound reduced to a repeated computation of 100th order determinants. In addition matrix elements $F_{ij}(E)$ has to be recounted for every energy E. Such a procedure requires a lot of computer time.

At the same time the KKR-equation is free from these two drawbacks. In KKR-method one again has to solve the determinant equation that is analogous to equation (1). But firstly, the matrix elements of the KKR-equation are decomposed into the potential and structural parts. The last one does not depend on E so, for a given crystal it is obtained only once. And the potential part, which depends on crystal potential and E, is calculated quickly and easily. Secondly, the order of the KKR determinant equation is much lower than in APW-method: the trial functions in KKR-method are spherical harmonics $Y_{lm}(\mathbf{r})$, and for every atom in the unit cell it is sufficient to take 9 or maximum – 16 trial functions, which compares favourably with 30–50 trial functions in APW-method. So, for calculations of multiatomic crystals KKR-method is preferable. Pseudoinverse matrix can be used to get in APW-method equations of the KKR-type.

Let us use the well-known equality

$$\frac{2l + 1}{4\pi} P_l(i, j) = \sum_{m=-l}^{m=l} \bar{Y}_{lm}(i) Y_{lm}(j),$$

where $Y_{lm}(i) \equiv Y_{lm}(\mathbf{k}_i)$ is the lth spherical harmonic corresponding to the vector $\mathbf{k}_i$. If there are $l_{\max}$ terms in sum (4) ($l = 0, 1, \ldots l_{\max} - 1$), then we designate $p = l_{\max}^2$.

Let us introduce a rectangular matrix A:

$$A_{lm,i} = 4\pi R j_l(k_i R) \bar{Y}_{lm}(i). \tag{6}$$

There is a double index for rows: l runs from 0 to $l_{\max} - 1$ and for a fixed l m runs from $-l$ to l; as a result there are p rows in matrix A; the index i runs from 1 to n.

Matrix A acts from R^n into R^p; the typical n values are about 100 and the typical p values are about: 10 for KKR-method and 100 for APW-method. Let us suppose that $p < n$.

We define a quadratic $p \times p$ diagonal matrix $L(E)$

$$L_{lm,l'm'}(E) = \delta_{ll'} \delta_{mm'} L(u_l),$$

where the diagonal matrix elements are logarithmic derivatives (5). Then it is easy to see that the expression (4) can be treated as (i, j)-matrix element of a triple production:

$$F_{ij}(E) = (A^* L(E) A)_{ij},$$

where A^* is matrix transposed and conjugated to matrix A. If $n \times n$ quadratic matrices J and M with matrix elements (2) and (3) are introduced the determinantal equation (1) can be rewritten as a vectoral equation:

$$[M + A^* L(E) A] \cdot \mathbf{u} = \lambda \cdot J\mathbf{u}, \quad \mathbf{u} \in R^n. \tag{7}$$

We have to find such a value of the parameter E that belongs to the set of eigenvalues of equation (7).

The matrix J is nonnegative and, hence, all eigenvalues of equation (7) are real. As soon as the parameter E value, for which the diagonal matrix $L(E)$ has been calculated, coincides with one of the equation (7) eigenvalues, we receive one of the system eigenenergies. The components of the corresponding eigenvector $\mathbf{u} = \{\mathbf{u}_i\}_1^n$ define the wave function. Let $\{E, \mathbf{u}\}$ be a solution of equation (7). If $\mathbf{u} \in \mathrm{Car}\ A$ (see Appendix), then

$$A\mathbf{u} = g \neq 0, \quad g \in R^p, \quad \mathbf{u} = A^{-1} g.$$

Multiplying equation (7) by $(A^*)^{-1} \equiv (A^{-1})^*$ and using equation (A5) we get:

$$[(A^*)^{-1} M A^{-1} + L(E)]g = \lambda (A^*)^{-1} J A^{-1} g. \tag{8}$$

Let as define

$$\tilde{M} = (A^*)^{-1} M A^{-1}, \quad \tilde{J} = (A^*)^{-1} J A^{-1}. \tag{9}$$

Then finally we have the vectoral equation

$$(\tilde{M} + L(E))g = \lambda \tilde{J} g. \tag{10}$$

and the determinantal equation

$$\det |\tilde{M} + L(E) - E\tilde{J}| = 0. \tag{11}$$

Equations (10) and (11) have some advantages over equations (1) and (7). The first – a comparative simplicity of matrix elements construction: though the calculation of the matrices $\tilde{M}$ and $\tilde{J}$ is a complicated problem, they do not depend on E and hence they can be calculated only once. Matrices $\tilde{M}$ and $\tilde{J}$ are analogous to the structural part of the KKR-equation which does not depend either on crystal potential nor on the energy E. The potential part of the equations is given by the diagonal matrix $L(E)$ and it is calculated without any difficulties.

The second important characteristic of equations (10) and (11), that completes their similarity to the KKR-type equations, is the $p \times p$ dimension [but not $n \times n$ as for equations (1) and (7)].

Here a remark should be made. Equation (11) is derived from equation (1) using a set of identities, so it is not at all necessary that equation (11) will give true results at small $l_{\max}$, when it is known that equation (1) well describes the energy spectrum of the system only at values of $l_{\max}$ about 10. Preliminary calculations with the empty-lattice test shows that even for $l_{\max} = 5$–7 precision of the obtained eigenenergies is not sufficient. Thus, if numerical calculations corroborate that in equation (11) $l_{\max}$ value about 10 has to be used, there will be no reduction of the dimension of the equation under consideration. Moreover, the dimension will increase, e.g. for monoatomic crystal it will increase from 50 [the number of the usually used APW's in equation (1)] to 100 ($l^2_{\max} = 100$).

Our hopes are for linear APW-method (LAPW) [4]. We think that for this method small $l_{\max}$ value about 3–4 can be used because its l-convergence is better than for APW-method. The LAPW-method can be reformulated in a l-representation analogously to what has been done here for APW-method; these results would be presented in a next publication.

3. A COMMENT

If the eigenvector $\mathbf{u}$ in the equation (7) belongs to the carrier of the matrix A, then the corresponding eigenvalue of equation (7) is equal to one of the eigenvalues of the equation (8). There can be such solutions of the latter equation that the corresponding vector $\mathbf{u}$ would not completely belong to the carrier of the matrix A, e.g.:

$$\mathbf{u} = \mathbf{u}_c + \mathbf{u}_k, \quad \text{where} \quad \mathbf{u}_c \in \text{Car } A, \mathbf{u}_k \in \text{Ker } A, \tag{12}$$

or

$$\mathbf{u} = \mathbf{u}_k. \tag{13}$$

It is impossible to express such a vector as $A^{-1}g$ (see Appendix) and, hence to transform the equation (7) into the equation (8).

It is well-known that in the frame of APW based methods more eigenenergies can be obtained than in the frame of KKR based methods, i.e. when using as trial functions a set of spherical harmonics Y_{lm}. Equalities (12) and (13) only describe, in a vectoral form, the additional solutions of APW-method. Some special problems connected with the different number of the solutions of equations (7) and (11) would be discussed in a following publication.

4. THE KKR-METHOD

With the use of the pseudoinverse matrices theory new interesting equations for the KKR-method can be derived.

Let the well-known determinantal KKR-equation [3] be the starting point:

$$\det \left| A_{lm,l'm'} + \kappa \delta_{ll'} \delta_{mm'} \frac{n_l(\kappa R) L(u_l) - n_l'(\kappa R)}{j_l(\kappa R) L(u_l) - j_l'(\kappa R)} \right| = 0, \tag{14}$$

where $\kappa = \sqrt{E}$, $n_l(\kappa R)$ is spherical Neuman function,

$$A_{lm,l'm'} = -\frac{(4\pi)^2 i^{(l-l')}}{\Omega_0 j_l(\kappa R) j_{l'}(\kappa R)} \times \sum_{i=1}^{n} \frac{j_l(k_i R) j_{l'}(k_i R) \bar{Y}_{lm}(i) Y_{l'm'}(i)}{k_i^2 - E} - \kappa \delta_{ll'} \delta_{mm'} \frac{n_l(\kappa R)}{j_l(\kappa R)},$$

$R, j_l, L(u_l), \Omega_0, Y_{lm}$ and k_i were defined in the previous section. The dimension of the determinant equation (14) is $p \times p$ ($p = l^2_{\max}$).

Rearranging the terms in equation (14), which contain the Kroneker symbols, and using the well-known equality for Wronskian we get

$$- \frac{\delta_{ll'} \delta_{mm'}}{R^2 j_l^2(\kappa R)[L(u_l) - L(j_l(\kappa R))]}.$$

Then the equation (14) can be rewritten as

$$\det \left| \left[(4\pi)^2 R^2 \sum_{i=1}^{n} \frac{j_l(k_i R) j_{l'}(k_i R) \bar{Y}_{lm}(i) Y_{l'm'}(i)}{k_i^2 - E} - \frac{\delta_{ll'} \delta_{mm'} \Omega_0}{L(u_l) - L(j_l(\kappa R))} \right] \frac{i^l}{j_l(\kappa R)} \frac{i^{-l'}}{j_{l'}(\kappa R)} \right| = 0.$$

It is clear that in this equation the factors out of the square brackets are unsubstantial.

To transform the expression in the square brackets the rectangular matrix A defined previously [see (6)] is

used and two square diagonal matrices are introduced. Namely, the $p \times p$ dimension $\tilde{L}(E)$:

$$(\tilde{L}(E))_{lm,l'm'} = \frac{\delta_{ll'}\delta_{mm'}}{\Omega_0}[L(u_l) - L(j_l(\kappa R))], \quad (15)$$

and the $n \times n$ dimension matrix $K(E)$:

$$K(E) = \text{diag}\,(k_i^2 - E) = K^2 - EI_n, \quad (16)$$

where $K^2 = \text{diag}\,(k_i^2)$, and I_n is a unit matrix in the space R^n.

Then the latter determinantal equation can be rewritten as:

$$\det|AK^{-1}(E)A^* - \tilde{L}^{-1}(E)| = 0,$$

or in the vectoral form:

$$AK^{-1}(E)A^*f = \tilde{L}^{-1}(E)\mathbf{f}, \quad \mathbf{f} \in R^p.$$

Thus, such a value of E is to be found that the latter vectoral equation will be satisfied for some vector $\mathbf{f} \in R^p$. It is clear that the same E will satisfy an equation with the inverse matrices (or with a pseudo-inverse matrix if some of the $p \times p$ matrices in this equation is degenerated). Then

$$(A^*)^{-1}K(E)A^{-1}\mathbf{f} = \tilde{L}(E)\mathbf{f}, \quad \mathbf{f} \in R^p, \quad (17)$$

where A^{-1} is the matrix pseudoinverse to A.

There are two possibilities now.

The first, we can get a KKR-equation in Ziman's form [5]. To do this let us define a nonzero vector $\mathbf{u} = A^{-1}\mathbf{f}$. Multiplying equation (17) by A^* and using the fact that in accordance with equality (A6) the matrix $A^*(A^*)^{-1}$ is an orthogonal projector on the matrix A carrier Car A, we can get

$$K(E)\mathbf{u} = A^*\tilde{L}(E)A\mathbf{u}, \quad (18)$$

or in the determinantal form

$$\det\left|(k_i^2 - E)\delta_{ij} - \frac{4\pi}{\Omega_0}R^2\sum_{l=0}(2l+1)P_l(i,j) \times j_l(k_iR)j_l(k_jR)[L(u_l) - L(j_l(\kappa R))]\right| = 0,$$

the well-known KKRZ-equation.

Again, as is mentioned in the Comment, only those solutions of equation (18) whose eigenvectors belong to the carrier of the matrix A would be solutions of equation (17). But, there could be another solution of equation (18) where eigenvectors have the form (12) or (13).

The second, starting from the equation (17) we can choose another course which leads to very interesting new results.

In fact, the equation (17) contains all the information, it is necessary only to rearrange its terms taking into account the definition (16). Then the equation (17) takes the form

$$[(A^*)^{-1}K^{-2}A^{-1} - \tilde{L}(E)]\mathbf{f} = E(AA^*)^{-1}\mathbf{f}, \quad \mathbf{f} \in R^p. \quad (19)$$

Undoubtedly this equation is of practical interest: its dimension is $p \times p$ and matrices $(A^*)^{-1}K^2A^{-1}$ and $(AA^*)^{-1}$ do not depend either on the crystal potential or on the parameter E, hence, for a given crystal they can be calculated only once; the potential part of the equation is only the diagonal matrix $\tilde{L}(E)$ and it is calculated easily.

As a whole the equation (19) has the same structure as the equation (10). It is rather easy to construct the matrices in this equation. The most complicated part is to find out all eigenvalues and eigenvectors of the small dimensional $p \times p$ symmetrical matrix AA^*; this work has to be done only once. The numerical calculations has to be done to estimate how small would be $p = l_{\max}^2$. A small value for $l_{\max}$ in equation (19) is more probable on account of equivalence of the equations (19) and (14).

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APPENDIX

The pseudo-inverse matrix

A pseudoinverse matrix is a matrix that is inverse to any degenerate matrix. The most general example of a degenerate matrix is a rectangular matrix that transforms a space R^n with a dimension n into a space R^p with a dimension p where $n > p$:

$$A = (A_{ij}), \quad i = 1, \ldots, p, \quad j = 1, \ldots, n,$$

$$A: R^n \to R^p, \quad n > p.$$

Without any restriction of the generality one may assume that the rank of the matrix A is p. Then

this matrix transforms n linear independent vectors from any R^n-basis into p linear independent vectors of R^p space. Hence, some subspace of the R^n space is transformed into zero. This subspace of the space R^n is called the kernel of the matrix — Ker A. If we interpret the rows of the matrix A as p vectors of the space R^n, it is clear, that these vectors are linear independent and so the p-dimensions subspace can be span on these vectors. Then the orthocomplementation to this subspace is exactly the kernel of the matrix A: matrix A would transform all the vectors from the orthocomplementation (and only these vectors) into zero. The dimension of Ker A is equal to $n-p$.

The linear subspace spanned on the p row-vectors of the matrix A is called the carrier of matrix — Car A: R^n = Ker $A \oplus$ Car A.

The matrix A transforms the vectors from Car A into nonzero vectors of the space R^p. It is clear, that the pseudoinverse matrix to A must be defined as the matrix that transforms R^p onto the subspace Car A, since only in this part of the space R^n the one-valued transformation inverse to A can be determined. In the following we will give the natural definition to a pseudoinverse matrix and we will mark it as ordinary inverse matrix — A^{-1}.

Let us introduce a matrix A^* that is conjugate to A. We may obtain it from A by transposition and complex conjugation of all matrix elements: $A^*_{ij} = \bar{A}_{ji}$. Then matrix A^* is acting from R^p in R^n. We will show below that actually A^* transforms R^p onto Car A.

Now we can give the definition of two Hermitian matrix:

$$N = A^*A\colon R^n \to R^n,$$

$$P = AA^*\colon R^p \to R^p.$$

The matrices N and P are nonnegative. All their eigenvalues are not less than zero. From the well-known theorem the ranks of matrices N and P are equal to the rank of A and hence are equal to p. It means that all eigenvalues of matrix P are positive:

$$P\mathbf{f}^{(i)} = \alpha_i \mathbf{f}^{(i)}, \quad \alpha_i > 0, \quad i = 1, 2, \ldots, p,$$

$$\mathbf{f}^{(i)} \in R^p.$$

It follows, then, that matrix A^* acts from R^p onto Car A: if matrix A^* would transform any vector $\mathbf{f} \in R^p$ into Ker A, then applying matrix A to $A^*\mathbf{f}$ we would obtain zero, which is impossible.

Only p eigenvalues of matrix N that has n nonnegative eigenvalues, are nonzero. Hence the rest of the $n-p$ eigenvalues equal zero exactly:

$$N\mathbf{u}^{(i)} = \beta_i \mathbf{u}^{(i)}, \quad \beta_i > 0, \quad i = 1, 2, \ldots, p,$$

$$\beta_{p+1} = \beta_{p+2} = \cdots = \beta_n = 0, \quad \mathbf{u}^{(i)} \in R^n.$$

It turns out that for all $i = 1, 2, \ldots, p$:

$$\alpha_i = \beta_i, \tag{A1}$$

$$A^*\mathbf{f}^{(i)} = \sqrt{\alpha_i}\mathbf{u}^i, \tag{A2}$$

$$A\mathbf{u}^{(i)} = \sqrt{\alpha_i}\mathbf{f}^{(i)}. \tag{A3}$$

Indeed multiplying the equality

$$P\mathbf{f}^{(i)} = AA^*\mathbf{f}^{(i)} = \alpha_i \mathbf{f}^{(i)},$$

by matrix A^*, we obtain: $A^*AA^*\mathbf{f}^{(i)} = \alpha_i A^*\mathbf{f}^{(i)}$. Otherwise, the vector $A^*\mathbf{f}^{(i)}$ is the eigenvector of matrix N and, hence, this vector is collinear to one of the vectors $\mathbf{u}^{(i)}$. Then the eigenvalue α_i is equal to the corresponding eigenvalue β_j. Since this argumentation is applicable to all α_i, we can numerate the eigenvalues of matrices P and N in such a way that equality (A1) would be fulfilled.

Then, $\|A^*\mathbf{f}^{(i)}\|^2 = (AA^*\mathbf{f}^{(i)}, \mathbf{f}^{(i)}) = \alpha_i$ from where the equality (A2) follows. If the matrix A acts on the equality (A2), we would obtain the equality (A3). It is convenient to choose the equality (A3) as the definition of the pseudoinverse matrix. The natural definition of the transformation that is inverse to (A3) will be:

$$A^{-1}\mathbf{f}^{(i)} = \frac{1}{\sqrt{\alpha_i}}\mathbf{u}^{(i)}, \quad i = 1, 2, \ldots, p.$$

The fact that the sets of the vectors $\{\mathbf{f}^{(i)}\}_1^p$, $\{\mathbf{u}^{(i)}\}_1^p$ form the ortho-normalized basis, allows us to write down a simple expression for the matrix elements A^{-1}_{ij} using the vectors $\mathbf{f}^{(l)}$ and $\mathbf{u}^{(l)}$ components:

$$A^{-1}_{ij} = \sum_{l=1}^{p} \frac{u_i^{(l)}\bar{f}_j^{(l)}}{\sqrt{\alpha_l}}, \quad i = 1, 2, \ldots, n; \quad j = 1, \ldots, p, \tag{A4}$$

here $u_i^{(l)}(f_j^{(l)})$ is i- (j-) component of the eigenvector $\mathbf{u}^{(l)}(\mathbf{f}^{(l)})$. The matrix A^{-1} acts from R^p onto Car A. For comparison let us write down the analogous expression for A^*_{ij}:

$$A^*_{ij} = \sum_{i=1}^{p} \sqrt{\alpha_i} u_i^{(l)} \bar{f}_j^{(l)}.$$

In those particular cases where the matrix A rank is p, matrix A^{-1} is the same as A^+ from [1]. To clear the situation let us show how matrices A^{-1} and A^* are related. If V is $n \times p$ matrix which columns are p vectors $\mathbf{u}^{(i)}/(\alpha_i)^{1/2}$, $i = 1, 2, \ldots, p$, it is easy to see that $A^{-1} = VV^*A^*$. Let us list some easily verified

equalities:

$$(AA^{-1})_{ij} = ((A^*)^{-1}A^*)_{ij} = \delta_{ij}, \quad i = 1, 2, \ldots, p, \quad j = 1, 2, \ldots, p, \tag{A5}$$

i.e. $AA^{-1} = (A^*)^{-i}A^* = I_p$ is a unit matrix in the space R^p. In the same time:

$$(A^{-1}A)_{ij} = (A^*(A^*)^{-1})_{ij} = \sum_{l=1}^{p} u_i^{(l)} \bar{u}_j^{(l)}. \tag{A6}$$

Matrix $A^{-1}A$ (as $A^*(A^*)^{-1}$) is orthogonal projector into Car A.