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CONCEPTS IN NUCLEAR SPIN DYNAMICS OF LIQUIDS. 2

(Presented by E. Lippmaa)

2. Basis systems

Making use of fundamental properties of algebraic operations described previously [1], one can establish general relationships between vectors and operators associated with the above-mentioned linear spaces. It is rational to use these general algebraic relationships foremost. However, in order to specify vectors and operators and to discuss particular experiments, one needs ordered sets of numbers — coordinates of vectors and matrices of operators. Thus, basis systems of vectors must be introduced in each linear space described in Sec. 1.1.

Two different kinds of orthogonal basis systems will be used throughout this work — the *I*-basis and the *A*-basis. Below we describe both kinds of basis systems and their physical meaning, using the two spin 1/2 system as an demonstrative example.

2.1. *A*-basis. The orthonormalized *A*-bases in space **C**, **O** and **H** of a *d*-level system refer to the particular spin system under study. If  $H_0$  denotes the static Hamiltonian of this system, then its *A*-basis in **C** is the orthonormalized set of eigenvectors  $|a_m\rangle \in \mathbf{C}$ ,  $m=1, 2, \dots, d$ , of  $H_0$ :

$$H_0|a_m\rangle = \omega_m^0 |a_m\rangle. \quad (2.1)$$

The corresponding orthonormalized *A*-basis in the space **O** is given by the following set of  $d^2$  linear operators

$$A_{mn} = |m\rangle\langle n|, \quad (m, n=1, 2, \dots, d). \quad (2.2)$$

These basis operators form an orthonormal set of eigenvectors of the corresponding static Superhamiltonian  $\mathcal{H}_0$  of the spin system under study:

$$\mathcal{H}_0 A_{mn} = -i\omega_{mn}^0 A_{mn}, \quad (2.3)$$

where the so-called transition frequencies

$$\omega_{mn}^0 = \omega_m^0 - \omega_n^0 \quad (2.4)$$

are subject to the Ritz relationships

$$\omega_{mm}^0 = 0, \quad (2.5)$$

$$\omega_{nm}^0 = -\omega_{mn}^0, \quad (2.6)$$

$$\omega_{mk}^0 + \omega_{kn}^0 = \omega_{mn}^0. \quad (2.7)$$

The matrix elements of the operator  $A_{mn}$  relative to the *A*-basis of **C** vanish except for the one on the intersection of *m*-th row and *n*-th column which possess the value 1. Therefore, if one expands a linear operator



on  $\mathbf{C}$ , say the density operator  $P$ , in terms of the  $A$ -basis of  $\mathbf{O}$  as shown by Eq. (2.8)

$$P = \sum_m \sum_n \pi_{mn} A_{mn}, \quad (2.8)$$

one gets for the coordinates of the vector  $P \in \mathbf{O}$

$$\pi_{mn} = (P, A_{mn}) = \langle a_m | P | a_n \rangle \quad (2.9)$$

the matrix elements of the linear operator  $P$  calculated relative to the  $A$ -basis of  $\mathbf{C}$ .

Some properties of the basis operators  $A_{mn}$  are given by Eq. (2.10), (2.11)

$$A_{mm}^\dagger = A_{mm}, \quad A_{mn}^\dagger = A_{nm}, \quad (2.10)$$

$$\text{tr } A_{mm} = 1, \quad \text{tr } A_{mn} = 0. \quad (2.11)$$

The matrix products between the basis operators  $A_{mn}$  vanish unless they have a «common level». In the latter case

$$A_{mk} A_{kn} = A_{mn}. \quad (2.12)$$

Starting from Eq. (2.12), one gets the following commutators of basis operators which do not vanish

$$[A_{mm}, A_{nn}] = A_{mn}, \quad (2.13)$$

$$[A_{mn}, A_{nm}] = A_{mm} - A_{nn}, \quad (2.14)$$

$$[A_{mk}, A_{kn}] = A_{mn}. \quad (2.15)$$

An hermitian operator on  $\mathbf{C}$ , like  $H_0$ , is specified: a) by the set of eigenvectors  $|a_m\rangle \in \mathbf{C}$  (by the unitary orientation of  $H_0$  in  $\mathbf{C}$ ) b) by the set of eigenvalues  $\omega_m^0$ . All hermitian operators (considered as vectors of  $\mathbf{O}$ ) with the same unitary orientation are located in a  $d$ -dimensional subspace  $\mathbf{O}_A \subset \mathbf{O}$  spanned by basis operators  $A_{mm}$ . They form the corresponding subspace  $\mathbf{H}_A \subset \mathbf{H}$  also spanned by  $A_{mm}$ . The traceless hermitian operators are located in the  $(d-1)$ -dimensional subspace  $\mathbf{O}_A^0 \subset \mathbf{O}_A$  and form the corresponding subspace  $\mathbf{H}_A^0 \subset \mathbf{H}$ . The latter is a  $(d-1)$ -dimensional commutative Lie subring  $\mathfrak{g}_A^0 \subset \mathfrak{su}(d)$  associated with the  $A$ -basis.

The transformation

$$H_T = \mathcal{C} H_0 = T H_0 T^{-1}, \quad T \in \mathbf{SU}(d) \quad (2.16)$$

generates a new hermitian operator  $H_T$  which has the same spectrum of energy levels  $\omega_m^0$  as  $H_0$ , and a different unitary orientation given by

$$|b_m\rangle = T |a_m\rangle. \quad (2.17)$$

If in Eq. (2.16)  $T$  runs through  $\mathbf{SU}(d)$ , one gets a class of equivalent hermitian operators (a spectral class) specified by the eigenvalue-spectrum  $\omega_m^0$ . Each possible spectral class has a representative  $H_0$  in subspace  $\mathbf{H}_A^0$ .

The transformations (2.16), (2.17) induce corresponding transformations in the adjoint representation

$$\mathcal{K}_T = \mathcal{C} \mathcal{K}_0 \mathcal{C}^{-1}, \quad (2.18)$$

$$B_{mn} = \mathcal{C} A_{mn} = |b_m\rangle \langle b_n|. \quad (2.19)$$



The bases  $|b_m\rangle \in \mathbf{C}$  and  $B_{mn} \in \mathbf{O}$  (the  $B$ -bases) are of the same kind as the corresponding  $A$ -bases, but they refer to  $H_T$  and to  $\mathcal{H}_T$ , respectively:

Note that the definition (2.1) of the  $A$ -basis in  $\mathbf{C}$  is not unique — one can multiply each  $|a_m\rangle$  with an arbitrary phase factor:

$$U|a_m\rangle = e^{-i\psi_m}|a_m\rangle. \quad (2.20)$$

In this case the basis operators  $A_{mn}$  will also be multiplied by a corresponding phase factor given by Eq. (2.21)

$$\mathcal{U}A_{mn} = e^{-i\psi_{mn}}A_{mn}, \quad (2.21)$$

where the angles

$$\psi_{mn} = \psi_m - \psi_n \quad (2.22)$$

are subject to Ritz relationships similar to Eq. (2.5) — (2.7).

Actually, Eq. (2.20) defines a unitary operator  $U \in \mathbf{O}_A$ , the unitary adjoint representation  $\mathcal{U}$  of which being given by Eq. (2.21). All such unitary operators  $U$  constitute the  $d$ -dimensional commutative Lie group  $\mathbf{G}_A \subset \mathbf{U}(d)$ .  $\mathbf{g}_A^0 = \mathbf{H}_A^0$  is the Lie ring of the unimodular subgroup  $\mathbf{G}_A^0 \subset \mathbf{G}_A$ . In Adiabatic NSD propagators which describe the motion in case  $H(t) = H_0 \in \mathbf{g}_A^0$  (Free Induction) belong to the subgroup  $\mathbf{G}_A^0 \subset \mathbf{SU}(d)$ . Since

$$\mathcal{U}H_0 = UH_0U^{-1} = H_0, \quad (2.23)$$

$\mathbf{G}_A$  is also the symmetry group of all hermitian operators  $H_0 \in \mathbf{H}_A^0$ . This is, of course, a trivial case of symmetry. In what follows we will speak about symmetrical hermitian operators and about their symmetry group  $\mathbf{G} \subset \mathbf{SU}(d)$  only in case  $H_0$  being degenerate and  $U$  running through  $\mathbf{G}$ .

It is to emphasize that an arbitrary unitary superoperator on  $\mathbf{O}$  is not necessarily the adjoint representation of a unitary operator on  $\mathbf{C}$ . Thus, an orthonormal basis in  $\mathbf{O}$  is not always an  $A$ -basis.

In order to introduce the  $A$ -basis of space  $\mathbf{H}$  which corresponds to the  $A$ -basis of  $\mathbf{O}$ , let us first define the following set of hermitian operators [2]

$$W_{mn} = (1/2)(A_{mm} + A_{nn}), \quad (2.24)$$

$$Z_{mn} = (1/2)(A_{mm} - A_{nn}), \quad (2.25)$$

$$X_{mn} = (1/2)(A_{mn} + A_{nm}), \quad (2.26)$$

$$Y_{mn} = -(i/2)(A_{mn} - A_{nm}). \quad (2.27)$$

We adopt the term single transition operators [3] for these operators. To each transition  $m \rightarrow n$  ( $m < n$ ) corresponds a set of mutually orthogonal single transition operators (2.24) — (2.27). As shown by Eq. (2.28) all single transition operators have equal norms

$$(W_{mn}, W_{mn}) = (Z_{mn}, Z_{mn}) = (X_{mn}, X_{mn}) = (Y_{mn}, Y_{mn}) = 1/2. \quad (2.28)$$

The traces of single transition operators are

$$\text{tr } W_{mn} = 1, \quad \text{tr } Z_{mn} = \text{tr } X_{mn} = \text{tr } Y_{mn} = 0. \quad (2.29)$$

If the space  $\mathbf{H}$  is decomposed into the direct sum

$$\mathbf{H} = \mathbf{H}_A + \mathbf{H}_\perp, \quad (2.30)$$

then the single transition operators  $X_{mn}, Y_{mn}, m, n = 1, 2, \dots, d; m < n$ ,



form an orthogonal basis of the  $d(d-1)$ -dimensional subspace  $\mathbf{H}_\perp$ , whereas  $W_{mn}$  and  $Z_{mn}$  are located in the subspace  $\mathbf{H}_A$ . However, the traceless single transition operators  $Z_{mk}$ ,  $Z_{kn}$  of a pair of connected transitions (e.g. of transitions which share a common level « $k$ ») are linearly dependent

$$Z_{mk} + Z_{kn} = Z_{mn}. \quad (2.31)$$

For this reason we put together the operators  $A_{mm} \in \mathbf{H}_A$  and  $X_{mn}$ ,  $Y_{mn} \in \mathbf{H}_\perp$  in order to form the  $A$ -basis of the space  $\mathbf{H}$ . Replacing the operators  $A_{mm}$  with a new set of  $(d-1)$ -mutually orthogonal basis operators which span the subspace  $\mathbf{H}_A^0$ , we get an orthogonal basis of  $\mathbf{H}^0$  associated with the original  $A$ -basis. These basis operators can be constructed as suitable linear combinations of single transition operators  $W_{mn}$  and  $Z_{mn}$ . The new basis in  $\mathbf{H}_A^0$  will be adapted to a Lie subring  $\mathfrak{g} \subset \mathfrak{su}(d)$  which governs a kind of experiments associated with  $A$ -basis.

The single transition operators (2.24)–(2.27) are related by the following set of commutation relations

$$-i[X_{mn}, Y_{mn}] = Z_{mn} \quad (2.32)$$

and cyclic permutations,

$$[W_{mn}, Z_{mn}] = [W_{mn}, X_{mn}] = [W_{mn}, Y_{mn}] = 0. \quad (2.33)$$

Eq. (2.32) tells that  $X_{mn}$ ,  $Y_{mn}$  and  $Z_{mn}$  span a 3-dimensional Lie subring  $\mathfrak{g}_L(mn) \subset \mathfrak{su}(d)$ . The Lie algebra of  $\mathfrak{g}_L(mn)$  is isomorphic with  $\mathfrak{so}(3)$  and  $\mathfrak{su}(2)$ . It is due to this isomorphism that selective excitation of a single transition leads to phenomena well known in the dynamics of single-spin 1/2 system.

Any two single transition operators which belong to different transitions commute unless they share a common level. In the latter case we have [2]

$$-i[X_{mk}, X_{kn}] = (1/2)Y_{mn}, \quad (2.34)$$

$$-i[X_{mk}, Y_{kn}] = -(1/2)X_{mn}, \quad (2.35)$$

$$-i[Y_{mk}, X_{kn}] = -(1/2)X_{mn}, \quad (2.36)$$

$$-i[Y_{mk}, Y_{kn}] = -(1/2)Y_{mn}. \quad (2.37)$$

To these equations we add the following two

$$\mathcal{K}_0 X_{mn} = -i[H_0, X_{mn}] = \omega_{mn}^0 Y_{mn}, \quad (2.38)$$

$$\mathcal{K}_0 Y_{mn} = -i[H_0, Y_{mn}] = -\omega_{mn}^0 X_{mn}, \quad (2.39)$$

which show that the adjoint representation  $\mathcal{K}_0$  of  $H_0$  on  $\mathbf{H}$  does not possess eigenvectors in  $\mathbf{H}_\perp$ , but there are invariant planes spanned by  $X_{mn}$ ,  $Y_{mn}$ . To each transition corresponds an invariant plane of  $\mathcal{K}_0$ .

In applying the transformation (2.21) to operators of the  $A$ -basis of  $\mathbf{H}$ , we get

$$\mathcal{U}A_{mm} = A_{mm}, \quad (2.40)$$

$$\mathcal{U}X_{mn} = \cos \psi_{mn} X_{mn} + \sin \psi_{mn} Y_{mn}, \quad (2.41)$$

$$\mathcal{U}Y_{mn} = -\sin \psi_{mn} X_{mn} + \cos \psi_{mn} Y_{mn}. \quad (2.42)$$

Therefore, the plane  $X_{mn}$ ,  $Y_{mn} \in \mathbf{H}_\perp$  of a typical transition is a rotation



plane. The orthogonal adjoint representation  $\mathcal{U}$  of the unitary operator  $U \in \mathbf{G}_A$  rotates the vectors of this plane by the angle  $\psi_{mn}$ .

The physical meaning of  $A$ -bases in Adiabatic NSD is in that they induce a decomposition of spaces  $\mathbf{C}$ ,  $\mathbf{O}$  and  $\mathbf{H}$  into subspaces which are invariant relative to propagators of the subgroup  $\mathbf{G}_A^0 \subset \mathbf{SU}(4)$ . This is the dynamical group for experiments like Free Induction. If relaxation is sufficiently weak, the Free Induction Decay experiments (the FT NMR spectra) can also be described in terms of  $A$ -bases of Liouville spaces.

If the Hamiltonian, the superoperator of relaxation [4], the density operator and the observable are explained in terms of  $A$ -basis, then the dynamical relationships one gets do not depend upon the nature of the spin system under study or upon particular interactions of this system. In order to correlate the laws of such Abstract NSD with actual experiments (e.g. to study possible physical realizations of the Abstract NSD), one must establish a correspondence between the  $A$ -basis and another basis of Liouville spaces build-up with the help of single spin operators — the  $I$ -basis. In principle, the whole dynamical problem could be studied in terms of the  $I$ -basis. Provided this is done, one can speak about the direct method in the theory of NMR [5-8]. We do not mean that the direct method introduces an «economy of thinking» in general. We will study the dynamical relationships of the Abstract NSD in terms of suitable  $A$ -bases. Then the physical interpretation of these relationships in terms of the  $I$ -basis will be considered as selected «static» topics.

**2.2.  $I$ -basis.** The  $I$ -basis of a many-spin system [9] is defined with reference to the laboratory coordinate system  $\vec{e}_j \in \mathbf{V}$ , and experiences an orthogonal (space  $\mathbf{H}$ ) or unitary (space  $\mathbf{O}$ ) transformation when this system rotates. The  $I$ -basis also refers to the composition of the spin system under study. Below the build-up of the  $I$ -basis of two spin 1/2 systems is demonstrated.

The  $I$ -basis of 4-dimensional Liouville spaces  $\mathbf{O}(\lambda)$  and  $\mathbf{H}(\lambda)$  of a single spin number  $\lambda$  ( $\lambda=1,2$ ) of the two-spin system is composed of single spin operators  $I_0(\lambda) = (1/2)E(\lambda)$ ,  $I_x(\lambda)$ ,  $I_y(\lambda)$  and  $I_z(\lambda)$ . The correspondence between the latter three operators and the laboratory coordinate system is established by Eq. (1.13). Note that Eq. (1.15) remains valid for all four single spin operators. Since

$$[I_0(\lambda), I_j(\lambda)] = 0, \quad (2.43)$$

$$-i[I_x(\lambda), I_y(\lambda)] = I_z(\lambda) \quad (2.44)$$

and cyclic permutations, the single spin space  $\mathbf{H}(\lambda)$  is a representation of the Lie algebra  $\mathfrak{u}(2)$ , whereas the 3-dimensional subspace  $\mathbf{H}^0(\lambda)$  spanned by  $I_j(\lambda)$  with  $j=x, y, z$  is a representation of  $\mathfrak{su}(2)$  and  $\mathfrak{so}(3)$ .

Unitary unimodular operators  $D(\lambda)$  on space  $\mathbf{C}(\lambda)$  form a representation of  $\mathbf{SU}(2)$ . The adjoint representation  $\mathfrak{D}(\lambda)$  of  $D(\lambda)$  on  $\mathbf{O}(\lambda)$  and  $\mathbf{H}(\lambda)$  does not change the operator  $I_0(\lambda)$  but rotates the other single spin operators. If one establishes such a one-one correspondence between the rotations of laboratory coordinate system and the superoperators  $\mathfrak{D}(\lambda)$  that Eq. (1.13) remains valid for transformed quantities, one gets a representation of  $\mathbf{SO}(3)$  on spaces  $\mathbf{O}^0(\lambda)$  and  $\mathbf{H}^0(\lambda)$ .

The  $I$ -basis of Liouville spaces  $\mathbf{O}$  and  $\mathbf{H}$  of two-spin 1/2 systems is formed by direct products of single spin operators  $I_j(\lambda)$  of both nuclei  $\lambda=1, 2$ :

$$I_{jk} = I_j(1) \times I_k(2) \in \mathbf{O}, \mathbf{H}, \quad (j, k=0, x, y, z). \quad (2.45)$$



The term basic spin tensors (of two-spin 1/2 systems) will be used for the hermitian operators (2.45).

The  $I$ -basis defined by Eq. (2.45) is orthogonal yet not normalized. Indeed

$$(I_{jk}, I_{jh}) = (I_j(1), I_j(1)) (I_h(2), I_h(2)) = 1/4. \quad (2.46)$$

One gets an orthonormalized  $I$ -basis by replacing the basic spin tensors (2.45) with the corresponding normalized basic spin tensors  $2I_{jk}$ .

According to Eq. (2.47),

$$\text{tr } I_{jk} = (\text{tr } I_j(1)) (\text{tr } I_h(2)) = \delta_{jk}, \quad (2.47)$$

the operator  $I_{00} = (1/4)E$  spans the 1-dimensional subspaces  $\mathbf{O}_E$  and  $\mathbf{H}_E$ , whereas the other basic spin tensors span the 15-dimensional subspaces  $\mathbf{O}^0$  and  $\mathbf{H}^0$  of traceless operators.

Such unimodular unitary operators  $D \in \text{SU}(4)$  on space  $\mathbf{C}$  which are built-up as direct products

$$D = D(1) \times D(2) \in \text{SU}(4) \quad (2.48)$$

of the above-mentioned operators  $D(\lambda)$  on  $\mathbf{C}(\lambda)$  constitute the Lie group  $\text{SU}(2) \times \text{SU}(2)$ , a 6-dimensional subgroup of the 15-dimensional Lie group  $\text{SU}(4)$ . The adjoint representation  $\mathfrak{D}$  of the operator (2.48) on Liouville spaces  $\mathbf{O}$  and  $\mathbf{H}$  is also a direct product of the corresponding single spin superoperators  $\mathfrak{D}(\lambda)$  on  $\mathbf{O}(\lambda)$  and  $\mathbf{H}(\lambda)$ :

$$\mathfrak{D} = \mathfrak{D}(1) \times \mathfrak{D}(2). \quad (2.49)$$

This means, in particular, that

$$\mathfrak{D}I_{jk} = \mathfrak{D}(1)I_j(1) \times \mathfrak{D}(2)I_h(2). \quad (2.50)$$

Thus, the single spin spaces in Eq. (1.3), (1.4) transform independently as do the single spin spaces in Eq. (1.2) if the operators (2.48) are applied.

The Liouville spaces of two-spin 1/2 systems decompose into a direct sum of subspaces which are invariant (and irreducible) with respect to the adjoint representation of  $\text{SU}(2) \times \text{SU}(2)$ . One gets this decomposition on the basis of Eq. (2.50) by noting that the superoperators (2.49) do not cause a change of single-spin operators  $I_0(\lambda)$ ,  $\lambda=1, 2$ . So in case of, say, space  $\mathbf{H}$  we have the following decomposition

$$\mathbf{H} = \mathbf{H}_E \dot{+} \mathbf{H}^{(1)}(1) \dot{+} \mathbf{H}^{(1)}(2) \dot{+} \mathbf{H}^{(2)}(1, 2). \quad (2.51)$$

In Eq. (2.51) the 3-dimensional subspaces  $\mathbf{H}^{(1)}(1)$  and  $\mathbf{H}^{(1)}(2)$  are spanned by  $I_{j0}$  and  $I_{0j}$ , ( $j=x, y, z$ ), respectively. The 9-dimensional subspace  $\mathbf{H}^{(2)}(1, 2)$  is spanned by basic spin tensors  $I_{jk}$  with  $j, k=x, y, z$ .

Such unitary operators (2.48) which carry out the same transformation in both single-spin spaces  $\mathbf{C}(\lambda)$ ,  $\lambda=1, 2$ , form the 3-dimensional subgroup  $\mathbf{G}_z \subset \text{SU}(4)$ , a representation of  $\text{SU}(2)$ . The adjoint representation of  $\mathbf{G}_z$  on  $\mathbf{H}$  and  $\mathbf{O}$  is a representation of  $\text{SO}(3)$  which describes the effect of rotation of laboratory coordinate system. With respect to this transformation the elements of subspaces  $\mathbf{H}^{(1)}(\lambda)$ ,  $\lambda=1, 2$ , are ordinary tensors of the first degree (ordinary vectors), whereas the elements of  $\mathbf{H}^{(2)}(1, 2)$  are ordinary tensors of the second degree. However, the adjoint representation of  $\mathbf{G}_z$  on  $\mathbf{H}^{(2)}(1, 2)$  is not irreducible. The subspace  $\mathbf{H}^{(2)}(1, 2)$  reduces into a 1-dimensional subspace of scalars, a 3-dimensional subspace of asymmetric tensors and a 5-dimensional subspace of irreducible symmetric tensors. The basis system of  $\mathbf{H}^{(2)}(1, 2)$  which induces this reduction is composed of irreducible spin tensors [10].

In order to make a difference in notation between unnormalized and



normalized basic spin tensors we supply the latter with an upper label — a number in brackets showing tensorial degree. Eq. (2.52), (2.53) bring examples of normalized basic spin tensors:

$$I_{z0}^{(1)} = 2I_{z0} = I_z(1) \times E(2) \in \mathbf{H}^{(1)}(1), \quad (2.52)$$

$$I_{zx}^{(2)} = 2I_{zx} = 2I_z(1) \times I_x(2) \in \mathbf{H}^{(2)}(1, 2). \quad (2.53)$$

The commutation relations between basic spin tensors of many-spin 1/2 systems are given in [9]. For a two-spin 1/2 system the main consequence of these relationships are: a) the subspaces  $\mathbf{H}^{(1)}(1)$  and  $\mathbf{H}^{(1)}(2)$  are representations of  $\mathfrak{su}(2)$ ; b) the operators of the noncommutative Lie rings  $\mathbf{H}^{(1)}(1)$  and  $\mathbf{H}^{(1)}(2)$  commute with each other; c) the direct sum  $\mathbf{H}^{(1)}(1) \dot{+} \mathbf{H}^{(1)}(2)$  is the infinitesimal ring of  $\mathbf{SU}(2) \times \mathbf{SU}(2)$ .

The total spin operators

$$I_j = I_{j0}^{(1)} + I_{j0}^{(2)} \in \mathfrak{g}_z, \quad (j = x, y, z), \quad (2.54)$$

span the infinitesimal ring  $\mathfrak{g}_z \subset (\mathbf{H}^{(1)}(1) \dot{+} \mathbf{H}^{(1)}(2))$  of the subgroup  $\mathbf{G}_z \subset \mathbf{SU}(2) \times \mathbf{SU}(2)$ . Of course,  $\mathfrak{g}_z$  is a representation of  $\mathfrak{su}(2)$ . The other 3-dimensional subspace  $\mathbf{H}_\Delta \subset (\mathbf{H}^{(1)}(1) \dot{+} \mathbf{H}^{(1)}(2))$  which is orthogonal and invariant with respect to  $\mathfrak{g}_z$ , is spanned by

$$\Delta_j = I_{j0}^{(1)} - I_{j0}^{(2)} \in \mathbf{H}_\Delta, \quad (j = x, y, z). \quad (2.55)$$

Expansion of hermitian operators of physical quantities in terms of normalized basic spin tensors allows one to specify these quantities. So, the operator of total nuclear magnetic dipole moment of the two-spin system in, say,  $x$ -direction  $M_x$  is the sum of corresponding individual magnetic moments of both nuclei:

$$M_x = \gamma_1 \tilde{I}_{x0}^{(1)} + \gamma_2 \tilde{I}_{x0}^{(2)} \in (\mathbf{H}^{(1)}(1) \dot{+} \mathbf{H}^{(1)}(2)), \quad (2.56)$$

where  $\gamma_1$  and  $\gamma_2$  denote the gyromagnetic ratios of nuclei number 1 and 2, respectively.

The density operator  $P$  of a two-spin 1/2 system is a positively definite hermitian operator on  $\mathbf{C}$  which satisfies the following conditions

$$\text{tr } P = 1, \quad (2.57)$$

$$1/4 \leq (P, P) \leq 1. \quad (2.58)$$

The hermitian operator  $P \in \mathbf{H}$  is specified by its unitary orientation in  $\mathbf{C}$  and by a set of positive eigenvalues (by the natural populations). The minimal length  $|P| = 1/2$  of the vector  $P$  is present in the state  $P = I_{00}$  which possess equal natural populations. The maximal length  $|P| = 1$  is realized only in case of pure quantum states like  $P = A_{mm}$ . In Adiabatic NSD only the unitary orientation of  $P$  does change if time proceeds.

Expanding  $P$  in terms of normalized basic spin tensors we have

$$P = I_{00} + P^{(1)}(1) + P^{(1)}(2) + P^{(2)}(1, 2) \in \mathbf{H}, \quad (2.59)$$

where

$$P^{(1)}(1) = \sum_j \pi_{j0} I_{j0}^{(1)} \in \mathbf{H}^{(1)}(1), \quad (2.60)$$

and

$$P^{(2)}(1, 2) = \sum_j \sum_k \pi_{jk} I_{jk}^{(2)} \in \mathbf{H}^{(2)}(1, 2), \quad (2.61)$$

are tensorial components of the density operator of the first and second



degree, respectively. The observed average value of the operator (2.56)

$$\langle M_x \rangle = (P, M_x) = \gamma_1 \hbar \pi_{x0} + \gamma_2 \hbar \pi_{0x} \quad (2.62)$$

is directly sensitive only to tensorial components (2.60) of the first degree.

In summing up what has been said about  $A$ -basis and  $I$ -basis it is instructive to note that both are defined with reference to a subgroup of  $SU(4)$  — the commutative subgroup  $G_A^0$  and the noncommutative subgroup  $SU(2) \times SU(2)$ , respectively. Both bases induce a decomposition of Liouville spaces into subspaces which are irreducible with respect to the adjoint representation of the corresponding subgroup of  $SU(4)$ . In turn, the reduction of the adjoint representation of a subgroup  $G \subset SU(4)$  defines an orthogonal basis of Liouville spaces which will be useful in the study of group aspects associated with  $G$ .

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V. SINIVEE

#### POHIMOISTEID VEDELIKE TUUMASPINNIDE DÜNAAMIKAS. 2

Tuumaspinnide dünaamikas on otstarbekohane kasutada üheaegselt kaht baasvektorite süsteemi —  $A$ -baasi ja  $I$ -baasi.  $A$ -baasi keeles väljendatud üldised dünaamilised seaduspärasused ei sõltu tuumaspinnide süsteemi konkreetsetest interaktsioonidest. Teisendus  $I$ -baasi keelde võimaldab anda nende seaduspärasuste füüsikalise interpretatsiooni igal konkreetsel juhul.

B. СИННІВЕЭ

#### ОСНОВНЫЕ ПОНЯТИЯ В ЯДЕРНОЙ СПИНОВОЙ ДИНАМИКЕ ЖИДКОСТЕЙ. 2.

В ядерной спиновой динамике целесообразно пользоваться одновременно двумя системами базисных векторов —  $A$ -базисом и  $I$ -базисом. Выраженные на языке  $A$ -базиса общие динамические закономерности не зависят от конкретных взаимодействий спиновой системы. Переход на язык  $I$ -базиса позволяет дать физическую интерпретацию этих закономерностей в каждом конкретном случае.