A Model of Control of an Equation for Two-Electron Interaction

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Abstract

Quantum Schrödinger equation, describing dynamical spin-interaction of two electrons with external magnetic field, is considered as an object for cybernetic research. Indeed, because of having a possibility to change external magnetic field, we can influence the interaction of particles. The algorithm of investigation of the algebraic structure of the spin-system is given. A specification of this algorithm is essentially connected with a control aspect. The spin-system is decomposed into six subsystems by using the found algebraic structure. Five from them are one-dimensional noninteract subsystems. Every from the latter has his own one-dimensional control.

1 Description of the system

Let us consider a Schrödinger equation for the spin-state $\mathcal{X}(t)$ of two spin-interacting electrons in an external inhomogeneous magnetic field [1]

$$i\hbar \frac{d}{dt} \mathcal{X}(t) = \hat{H}_s \mathcal{X}(t) \tag{1}$$

with the Hamiltonian $\hat{H}_s = A\vec{\sigma}_1 \cdot \vec{\sigma}_2 + \mu_1 \vec{\sigma}_1 \cdot \vec{B}_1(t) + \mu_2 \vec{\sigma}_2 \cdot \vec{B}_2(t)$, where $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are Pauli operators, $\vec{B}_1 = (B_{1x}, B_{1y}, B_{1z})$ and $\vec{B}_2 = (B_{2x}, B_{2y}, B_{2z})$ are magnetic inductions for the first and second particles, respectively.

For a matrix representation $\mathcal{X} = \|\mathcal{X}_{kn}\|_{k,n=1,2}$, dynamical equation (1) is transformed to

$$\dot{\mathcal{X}} = i\sigma_l \mathcal{X} \sigma_l^T + u_{1l}(t)\sigma_l \mathcal{X} + u_{2l}(t)\mathcal{X} \sigma_l^T,$$
(2)

where $\sigma_1 = i\sigma_x, u_{11} = -\mu_1 B_{11}/4A$ and analogously for $\sigma_2, \sigma_3, u_{12}, u_{13}, u_{21}, u_{22}, u_{23}$ and x, y, respectively; $\dot{\mathcal{X}} = d\mathcal{X}/d\tau$, $\tau = 4At/\hbar$. The functions $u_{kl}(t)$ are considered as control ones consisting of independent components.

System (2) has the first integral $|\mathcal{X}|^2 = \text{tr } \mathcal{X}\mathcal{X}^* = 1$, because of the spin-wavefunction is normed on unit. It is verified by direct calculation. The last means that all system trajectories are on a seven-dimensional sphere S^7 which is the space of states.

2 Constructing a Lie algebra of the system

The Lie algebra \mathcal{L} of system (2) is generated by vector fields $i\sigma_l \mathcal{X} \sigma_l^T$, $\sigma_j \mathcal{X}$, $\mathcal{X} \sigma_j^T$ (j = 1, 2, 3). It is verified by direct calculation that dim $\mathcal{L} = 15$ and vector fields

$$\sigma_l \mathcal{X} \sigma_l^T, \ \sigma_j \mathcal{X}, \ \mathcal{X} \sigma_j^T \ (l, j = 1, 2, 3) \tag{3}$$

Copyright © 1997 by Mathematical Ukraina Publisher. All rights of reproduction in any form reserved. form a basis of a linear space of the algebra \mathcal{L} . Moreover, it is obvious that $\mathcal{L} \sim \mathbf{su}(4)$ and consequently in accordance with [2] system (2) is completely controllable, because $\mathbf{su}(4)$ is a compact algebra. Inasmuch as the algebra $\mathcal{L} = \mathbf{su}(4)$ is simple, we consider the set $\mathfrak{N} = \mathcal{F}(S^7)\mathcal{L}$ being a $\mathcal{F}(S^7)$ modulus over the ring of real C^{∞} smooth functions defined on the manifold S^7 . The transition $\mathcal{L} \to \mathfrak{N}$ transforms the algebra \mathcal{L} into a set $V(S^7)$ of tangent smooth vector fields over the manifold S^7 . A first direct result of this step is a discovering of such a fact as the possibility to control system (2) by five controllings only instead of six ones, because $q_l(\mathcal{X})\sigma_l\mathcal{X} + p_l(\mathcal{X})\mathcal{X}\sigma_l^T = 0$ for vector field (3). But the main advantage of this step is the possibility to study different distributions on the set $\mathcal{L} = V(S^7)$ of vector fields, which turn out to be potential containers of information about the system structure.

3 Construction of decomposition structures of a distribution

It is shown in [3, 4] that an approach of the algebra of distributions into differentialgeometrical context is a comfortable and practical language for describing any dynamical system structures. Especially this approach is fruitful for control systems (a system may be represented in this form, because of universality and fundamental nature of cybernetics categories). It was usually to use specific parameters for analysis of symmetry structures of differential equations [5, 6]. But they were not considered as controllings. Usefulness of such a point of view is demonstrated in this work.

Analysis and synthesis of all possible structures of a dynamical control system and distribution structures \mathcal{L} , connected with them in a one-to-one correspondence, are described in [3, 4] and Appendix. The distribution structure is understood as a family of involutive distributions $\mathcal{L}_1, \mathcal{L}_2, \ldots, \mathcal{L}_r \subset \mathcal{L}$ being into certain relations among themselves and satisfing the Wonham–Hirschorn conditions (see Appendix). Unfortunatly, these distrubutions aren't known initially. In the work we suggest a way for finding distributions of system (2) from family (3). Of course, this way is dictated in general by concrete properties of system (2). Nevertheless, a basic pecularity of the way, independent of the concrete system, consists in forming the distributions from a finite or infinite family of vector fields set by the system, similarly to (3).

The structure is recurrently sought in several steps. It is possible to formulate them briefly in the following way.

Step 1. Let us choose any two vector-fields $L_1(\mathcal{X}), L_2(\mathcal{X})$ transversal to $\mathcal{B}(\mathcal{X}) =$ Span $\{\sigma_l \mathcal{X}, \mathcal{X} \sigma_l^T, l = 1, 2, 3\}$ and $[L_1(\mathcal{X}), L_2(\mathcal{X})] \in \mathfrak{N}_1 \mathcal{X} = \{L_1(\mathcal{X})L_2(\mathcal{X})\}_{\text{Lie}}$. The Wonham–Hirschorn conditions are held automatically, because $\mathfrak{N}_1(\mathcal{X}) + \mathcal{B}(\mathcal{X}) = T_{\mathcal{X}}S^7$ and dim $\mathcal{L}_1(\mathcal{X}) \bigcup \mathcal{B}(\mathcal{X}) = 0$.

Step 2. Let us choose the vector-field $L_3 \in \mathcal{B}$ and $L_3(\mathcal{X} \notin \mathfrak{N}_1(\mathcal{X}), [L_3(\mathcal{X}), \mathfrak{N}_1(\mathcal{X})] \subset \mathfrak{N}_2(\mathcal{X}) = \{\mathfrak{N}_1(\mathcal{X}), L_3(\mathcal{X})\}_{\text{Lie}}$, then the Wonham–Hirschorn conditions are held automatically because $\mathfrak{N}_2(\mathcal{X}) + \mathcal{B}(\mathcal{X}) \supseteq \mathfrak{N}_1(\mathcal{X}) + \mathcal{B}(\mathcal{X})$, i.e., $\mathfrak{N}_2(\mathcal{X}) + \mathcal{B}(\mathcal{X}) = T_{\mathcal{X}}S^7$ and $\dim \mathfrak{N}_2(\mathcal{X}) \cap \mathcal{B}(\mathcal{X}) = 1$, as $\mathfrak{N}_2(\mathcal{X}) \cap \mathcal{B}(\mathcal{X}) = \text{Span}; \{L_3(\mathcal{X})\}.$

Step 3–5. Analogously we can choose $\mathfrak{N}_3 = {\mathfrak{N}_2, L_4}_{\text{Lie}}, \mathfrak{N}_4 = {\mathfrak{N}_3, L_5}_{\text{Lie}}, \mathfrak{N}_5 = {\mathfrak{N}_4, L_6}_{\text{Lie}}$ with $L_4(\mathcal{X}) \notin \mathfrak{N}_2(\mathcal{X}), L_5(\mathcal{X}) \notin \mathfrak{N}_3(\mathcal{X}), L_6(\mathcal{X}) \notin \mathfrak{N}_4(\mathcal{X}), L_4, L_5, L_6 \in \mathcal{B}$. Their existence is guaranteed by the condition dim $\mathcal{B}(\mathcal{X}) = 5$. The Wonham–Hirschorn conditions are held authomatically likely to the step 2.

Finally we have a sequence $\mathfrak{N}_1 \subset \ldots \subset \mathfrak{N}_5$ satisfying the Wonham-Hirschorn conditions. This means (see Appendix) that we have a cascade-cascade decomposition of the structure with six subsystems. Indeed, after transformation of the state-vector

$$\begin{split} y_1 &= \frac{1}{2} \mid \varphi_- \mid^2, \quad y_2 = \frac{1}{2} \mid \varphi_+ \mid^2, \quad y_3 = \frac{1}{2} \mid \varphi_- \mid^2, \\ y_4 &= \frac{1}{2} \mid \varphi_+ \mid^2, \quad y_5 + iy_6 = \frac{1}{2}(\varphi_+^2 + \psi_-^2), \\ y_7 + iy_8 &= \frac{1}{2}(\varphi_-^2 + \varphi_+^2 - \varphi_+^2 - \varphi_-^2), \quad \varphi_\pm = \mathcal{X}_{21} \pm \mathcal{X}_{12}, \quad \psi_\pm = \mathcal{X}_{11} \pm \mathcal{X}_{22} \end{split}$$

and the control vector

$$\begin{cases} v_{1} = -Im(\bar{\phi}_{-}\psi_{-})(u_{11} - u_{21}) + Re(\bar{\phi}_{-}\psi_{+})(u_{12} - u_{22}) + \\ Im(\bar{\phi}_{-}\phi_{+})(u_{13} - u_{23}), \\ v_{2} = -Im(\bar{\phi}_{-}\phi_{+})(u_{13} - u_{23}) - Im(\bar{\phi}_{+}\psi_{+})(u_{11} + u_{21}) + \\ Re(\bar{\phi}_{+}\psi_{-})(u_{12} - u_{22}), \\ v_{3} = Im(\bar{\phi}_{-}\psi_{-})(u_{11} - u_{21}) - Re(\bar{\phi}_{+}\psi_{-})(u_{12} + u_{22}) - \\ Im(\bar{\psi}_{-}\psi_{+})(u_{13} - u_{23}), \\ v_{4} = -Re(\bar{\phi}_{-}\psi_{+})(u_{12} - u_{22}) + Im(\bar{\phi}_{+}\psi_{+})(u_{11} + u_{21}) + \\ Im(\bar{\psi}_{-}\psi_{+})(u_{13} - u_{23}), \\ v_{5} + iv_{6} = i[\phi_{-}\psi_{-}(u_{11} - u_{21}) - \phi_{-}\phi_{+}(u_{13} - u_{23}) + \\ \phi_{+}\psi_{+}(u_{11} + u_{21}) + \psi_{-}\psi_{+}(u_{13} + u_{23})], \end{cases}$$

$$(4)$$

the system (2) can be written in the form

$$\begin{cases} \dot{y}_1 = v_1, \ \dot{y}_2 = v_2, \ \dot{y}_3 = v_3, \ \dot{y}_4 = v_4, \ \dot{y}_5 = v_5, \ \dot{y}_6 = v_6, \\ \dot{y}_7 + i\dot{y}_8 = [\Delta + i[|\ \gamma \ |^2 + y_1^2 - y_4^2)]/\overline{\gamma}, \end{cases}$$
(5)

where $\Delta = \sqrt{\delta(\delta - 2 | \gamma |)(\delta - 2y_1)(\delta - 2y_4)}$, $\delta = y_1 + y_4 + |\gamma|$, $\gamma = y_5 + iy_6 + y_7 + iy_8$ and $\varphi_-^2 + \psi_+^2 \neq 0$. Directly from (4) one can verify the equality $v_1 + v_2 + v_3 + v_4 = 0$, i.e., first, there are only five really independent controllings in system (5) and, secondly, in this system there exists the first integral $y_1 + y_2 + y_3 + y_4 = 1$ (corresponding to $|\mathcal{X}|^2 = 1$ in system (2)). Therefore, the dimension of the state space is in fact equal to seven. If $\varphi_-^2 + \psi_+^2 = 0$, then system (5) is degenerated to four-dimensional one: $\dot{y}_2 = v_2$, $\dot{y}_3 = v_3$, $\dot{y}_5 = v_5$, $\dot{y}_6 = v_6$, because $y_1 = y_4$, $y_5 + iy_6 + y_7 + iy_8 = 0$ with control arguments being dependent. However, on the surface it is possible to use another transformation. For example, if $\varphi_-^2 + \varphi^2 \neq 0$, then as a possible variant, this transformation differs from preceeding one by the equalities $y_5 + iy_6 = (\varphi_+^2 + \psi_-^2)/2$, $v_5 + iv_6 = \phi_-\psi_+(u_{12} - u_{22}) - i\phi_-\phi_+(u_{13} - u_{23}) + \phi_+\psi_-(u_{12} - u_{22}) - i\psi_-\psi_+(u_{13} + u_{23})$ and the equation $\dot{y}_7 + i\dot{y}_8 = [\Delta + i(|\gamma|^2 + y_1^2 - y_3^2)]\overline{\gamma}$, $\Delta = \sqrt{\delta(\delta - 2|\gamma|)(\delta - 2y_1)(\delta - 2y_3)}$, $\delta = y_1 + y_3 + |\gamma|$. And so on under another possible degenerations.

<u>Remark.</u> As one can see from (5), the structure of system (2) is proved to be more rich, than one of the Lie algebra \mathcal{L} constructed above. It testifies in accodance with

the general theoretic investigations [3, 4] to the existence of additional relations between subdistributions $\mathfrak{N}_1, \ldots, \mathfrak{N}_5 \subset \mathcal{F}(S^7)\mathcal{L}$, the finding of which goes out the frames of the work.

The representation (5) facilitates a solution of some control problems. For example, the problem of maximization of a singlet component for a singlet-triplet mixture is solved more simple and this fact is important for researches of boson condensing in the super-conductivity problem.

Conclusions

Within classical algebraic analysis, a resolving structure is found wich is based on a direct sum of ideals [7, 8]. Therefore it is useful to analyze the modular structure of \mathcal{L} . Moreover, the modular approach allows us to analyze practically any structure, not only decompositions but quasidecompositions, pseudodecompositions, and so on. Moreover, classical algebraic analysis one allows to find a structure only but does not provide a structure synthesis by using feedback control. The modular structure approach resolves this problem.

Appendix

Let us consider a dynamical system with the control defined as a triplet of objects $\sum(X, \mathcal{E}, F)$, for which the diagram



is commuting. Here $\pi : \mathcal{E} \to X$ is a fiber bundle with the total manifold \mathcal{E} , dim $\mathcal{E} = n + m$ and base $X, dim X = n; \pi_X : TX \to X$ is a tangent bundle and $F : \mathcal{E} \to X$ is X a morphism [9]. All these maps and manifolds are supposed to be C^{∞} -smooth. Then for any system trajectories into a local chart $\{\mathcal{N}, x, u\} \in \mathcal{A}_{\mathcal{E}}$ from the total manifold atlas, the equation $\dot{x} = F(x, u)$ is obtained. The control functions u(t) are supposed piecewise differentiable with values from the set $\mathcal{N}_x = \mathcal{N} \cap \mathcal{E}_x$, dim $\mathcal{N}_x = m$.

Definition 1 Let vectors $F = col(\bar{F}^1, \ldots, \bar{F}^K)$, $x = col(\bar{x}^1, \ldots, \bar{x}^K)$, $u = col(u^1, \ldots, u^{K'})$ are broken up onto blocks and let us consider the corresponding blocks of matrices $\partial F/\partial x$, $\partial F/\partial u$, in which nonzero blocks substitute by units. Obtained $K \times K$ - and $K \times K'$ dimensional matrices (θ, Ξ) with zeroes and units we call the structure for system (6)
into the local chart $\{\mathcal{N}, x, u\} \in \mathcal{A}_{\mathcal{E}}$. If the local structure is the same for any chart $\{\mathcal{N}, x, u\} \in \mathcal{A}_{\mathcal{E}}$, then we use the term "structure" without "local". Matricis θ, Ξ are called
a state vector structure and a control vector structure (or U-structure), respectively.

Theorem 1 [4]. For system (6) the next statements are equivalent:

a) there exists a cascade-cascade decomposition structure (i.e., block-triangular decomposition in both the state vector and control-vector simultaneously); b) there exist factor-systems $\sum(X, \mathcal{E}, F) = \sum_0 (X_0, \mathcal{E}_0, F_0) \supset \sum_1 (X_1, \mathcal{E}_1, F_1) \supset \ldots \supset \sum(X_K, \mathcal{E}_K, F_K)$ defined by surjective submersies Φ_s, φ_s for which the commutative diagram is held;



c) there exists a sequence of involutive distributions $\mathcal{D}_1 \subset \ldots \subset \mathcal{D}_K \subset V(\mathcal{E})$, for which the Wonham-Hirschorn conditions $[\Delta^e(z), \mathcal{D}_s(z)] \subseteq \mathcal{D}_s(z) + \Delta^e_0(z)$, dim $\mathcal{D}_s(z) \cap \Delta^e_0(z) = m_s = \text{const}, \ \forall \{\mathcal{N}, z\} \in \mathcal{A}_{\mathcal{E}} \ (s = 1, \ldots, K) \ are \ held, \ where \ \Delta^e(z) = \{g(z) : g \in V(\mathcal{E}), T\pi(g(z)) = F(z)\}, \Delta^e_0(z) = \Delta^e(z) - \Delta^e(z) = \ker T\pi;$

d) there exists a sequence of involutive distributions $C_1 \supset \ldots \supset C_K \supset V(X)$, for which the Wonham-Hirschorn condition $[F(x, u), C_s(x)] \subseteq C_s(x) + \mathcal{B}(x, u)$, dim $\mathcal{B}(x, u)$ $\cap C_s(x) = m_s = \text{const}, \ \forall \{\mathcal{N}, x, u\} \in \mathcal{A}_{\mathcal{E}}(s = 1, \ldots, K) \text{ are held, where } \mathcal{B}(x, u) =$ $Span \left\{ \frac{\partial F(x, u)}{\partial u^{\nu}}, \nu = 1, \ldots, m \right\}$. Among distributions C_s, \mathcal{D}_s , relations ker $T\psi_s = C_s =$ $T\pi(\mathcal{D}_s) = T\pi$ ker $T\Psi_s$ are held, where $T\psi_s = T\varphi_s \circ T\varphi_{s-1} \circ \ldots \circ T\varphi_1, \ T\Psi_s = T\Phi_s \circ$ $T\Phi_{s-1} \circ \ldots \circ T\Phi_1 \ (s = 1, \ldots, K).$

Analogously it is possible to formulate statements for any dynamical control system structure. Further, some of such cases are formulated.

Theorem 2 [4]. Let for system (6) the conditions of Theorem 1 be held. Then the next statements are equivalent:

a) there exists parallel-parallel decomposition structure $\theta = \Xi = diag(1, ..., 1)$ (i.e., block-diagonal decomposition for both state and control vectors simultaneously);

b) the relations $[\mathcal{D}_s(z), \mathcal{D}_{s+1}(z)] \subseteq \mathcal{D}_s(z)(s = 1, ..., K, \mathcal{D}_{K+1} = V(\mathcal{E}), \forall \{\mathcal{N}, x, u\} \in \mathcal{A}_{\mathcal{E}})$ are true and for involutive $\mathcal{F}(\mathcal{E})$ -factor-distributions $\mathcal{M}_s(z) = \mathcal{D}_s(z)/\mathcal{D}_{s-1}(z)$ the Wonham-Hirschorn conditions $[\Delta^e(z), \mathcal{M}_s(z)] \subseteq \mathcal{M}_s(z) + \Delta^e_0(z), \dim \mathcal{M}_s(z) \cap \Delta^e_0(z) = m_s - m_{s-1} = \text{const}, \forall \{\mathcal{N}, z\} \in \mathcal{A}_{\mathcal{E}} (s = 1, ..., K + 1, \mathcal{D}_0 = 0)$ are held;

c) the relations $[\mathcal{C}_s(x), \mathcal{C}_{s+1}(x)] \subseteq \mathcal{C}_s(x)(s = 1, \dots, K, \mathcal{C}_{K+1} = V(X), \forall \{\mathcal{N}, x, u\} \in \mathcal{A}_{\mathcal{E}})$ are true and for involutive $\mathcal{F}(X)$ -factor-distributions $\mathcal{K}_s(x) = \mathcal{C}_s(x)/\mathcal{C}_{s-1}(x)$ the

conditions $[F(x, u), \mathcal{K}_s(x)] \subseteq \mathcal{K}_s(x) + \mathcal{B}(x, u), \text{ dim } \mathcal{B}(x, u) \cap \mathcal{K}_s(x) = m_s - m_{s-1} =$ const, $\forall \{\mathcal{N}, x, u\} \in \mathcal{A}_{\mathcal{E}}(s = 1, \dots, K + 1, \mathcal{C}_0 = 0)$ are satisfied.

Definition 2 The diagram of inclusions

is called cascadable if it can be represented in the form of a involutive distribution chain $\mathcal{R}_1 \subset \ldots \subset \mathcal{R}_q(q > K + 1)$ generated by different relations among $\{\mathcal{C}_s, \mathcal{P}_s, s = 1, \ldots, K\}$ with diagram inclusions among other ones). The constructing procedure of this chain is called cascading, the chain is called cascade.

Theorem 3 [3]. For the system (6) the next statements are equivalent:

a) there exists a cascade-cascade quasidecomposition structure (i.e., block-triangular partial decomposition for both state and control vectors simultaneously);

b) there exists a cascadable inclusion diagram (7) with the cascade of involutive distributions $\mathcal{R}_1 \subset \ldots \subset \mathcal{R}_{2K} \subset V(X)$, every of which is either \mathcal{C}_s or \mathcal{P}_s and for which Wonham-Hirschorn conditions $[F(x, u), \mathcal{C}_s(x)] \subseteq \mathcal{P}_s(x) + \mathcal{B}(x, u)$, dim $\mathcal{B}(x, u) \cap \mathcal{P}_s(x) =$ $m_s = \text{const}, \ \forall \{\mathcal{N}, x, u\} \in \mathcal{A}_{\mathcal{E}} \ (s = 1, \ldots, K) \ are \ held.$

And so on for other structures.

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