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ON CRYSTALLIZATION PROBLEM IN STATISTICAL CRYSTAL THEORY WITH SYMMETRIES OF COMPOSITE LATTICES

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Abstract Bifurcation theory methods under group symmetry conditions [6, 7] are applied to crystallization problem with composite lattices in statistical crystal theory. The obtained results are supported by RFBR-RA grant No. 07-01-91680.

Crystallization of liquid phase state in the case of composite lattice is described by the system of nonlinear integral equations with kernel depending on modulus of arguments difference [1], obtaining by the uncoupling of N.N. Bogolyubov equation hierarchy on second distribution function. Suppose that forming crystal molecules belong to M different classes and the number of i-th class molecules in the volume V is equal to N_i, $N=\sum_{i=1}^{M} N_i$

$$\frac{\partial F_i}{\partial q^\alpha}+\frac{1}{\theta v}\sum_{j=1}^{M} n_j \frac{\partial \Phi_{ij}(|q-q'|)}{\partial q^\alpha}F_{ij}(q,q')dq'=0, \quad q=(q^1,q^2,q^3) \qquad (1)$$

Here $\theta=kT$, k – Boltzman constant, T – temperature, $n_i=\frac{N_i}{N}$, $v=\frac{V}{n} \Rightarrow \frac{n_j}{v}=\frac{N_j}{V}=\frac{1}{v_j}$, $\Phi_{ij}(|q-q'|)=\Phi_{ji}(|q-q'|)$ – the potential energy of i-th and j-th molecule classes interaction which are disposed at the points q and q'.

Carrying out the approximation $F_{ij}(q,q')=F_i(q)F_j(q')G_{ij}(|q-q'|)$, $\lim\limits_{|q-q'|\to\infty} G_{ij}(|q-q'|)=1$; $G_{ij}(|q-q'|)=0$ at $|q-q'|\le a$, where $G_{ij}(|q-q'|)$ is radial distribution function of two types of particles, transform (1) to the form

$$\frac{\partial F_i(q)}{\partial q^\alpha} + \frac{1}{\theta v}\sum_{j=1}^{M} n_j \frac{\partial U_{ij}(q)}{\partial q^\alpha} F_i(q) = 0,$$

$$U_{ij}(q) = \int\limits_{(q')} \left\{ \int\limits_{\infty}^{|q-q'|} \frac{d\Phi_{ij}(r)}{dr} G_{ij}(r)dr \right\} F_i(q')dq'.$$

Setting $F_i(q) = \frac{1}{\lambda_i} \exp\left\{ -\frac{1}{\theta v} \sum\limits_{j=1}^{M} n_j \int\limits_{\infty}^{|q-q'|} \frac{d\Phi_{ij}(r)}{dr} dr \right\}$, where $\frac{1}{\lambda_i}$ is a constant not depending on coordinates and defining from the condition of density normalization $\lim_{V\to\infty} \frac{1}{V} \int F_i(q)dq = 1$, and $\rho_i(q) = \frac{1}{v_i} F_i(q) = \frac{1}{\lambda_i v_i} e^{u_i(q)}$ we obtain the system of nonlinear integral equations

$$\ln\{\lambda F_i(q)\} = u_i(q) = -\frac{1}{\theta} \sum_{j=1}^{M} \int \frac{1}{\lambda v_j} K_{ij}(|q-q'|) e^{u_j(q')} dq',$$

$K_{ij}(|q-q'|) = K_{ji}(|q-q'|) = \int\limits_{\infty}^{|q-q'|} \frac{d\Phi_{ij}(r)}{dr} G_{ij}(r)dr$, where $q = (q^1, q^2, q^3)$ are Cartesian coordinates. As far as $\frac{1}{v_i} = \frac{n_i}{v} = \frac{1}{Mv}$, the system of integral equations takes the form

$$u_i(q) + \frac{1}{Mv\theta\lambda} \sum_{j=1}^{M} \int K_{ij}(|q-q'|) e^{u_j(q')} dq' = 0. \tag{2}$$

As far as composite lattice consists of M identical sublattices here, like in [2], it is introduced the common constant of normalization λ.

First, give a brief introduction to crystallographic groups. It is know [3] that all symmetry groups of 3-dimensional homogeneous discrete space – spatial crystallographic groups – are three times periodic. The translations group $T = \{\mathbf{a} = m_1\mathbf{a}_1 + m_2\mathbf{a}_2 + m_3\mathbf{a}_3\}$, $m_i \in \mathbb{Z}$ propagates any point into $3D$-periodic system of points, that is a spatial lattice. Crystalline lattices are divided into 7 crystalline systems, that are called the syngonies. Bravais mathematically showed that for the crystals of 7 syngonies, 14 types of lattices are possible. Besides of translational symmetry the crystallographic groups are characterized by the point symmetry K – the aggregate of rotation and reflection operations being the symmetry of elementary cell. There are 32 point groups called the crystalline classes which are compatible with the translation group. However, the space crystallographic groups have new elements of symmetry that are absent in translation and point groups: screw displacements and glide reflections. Screw displacement is the translation with subsequent rotation at some angle around the translation axis. Glide reflection is the reflection in some plane with subsequent translation along this plane. Both indicated symmetry elements are formed by commuting elements; these elements themselves can be absent in crystallographic group.

Remark 1. Give the geometric interpretation of composite lattice. There are identical particles in the lattice nodes possessing the color symmetry of the point group K. For the nonsymmorphic group C_{2h}^5 of monoclinic syngony such particles may be interpreted as a ball, divided into 4 parts by two mutual perpendicular planes passing through the ball center, each part of the ball being colored into white or black. The translation group T propagates such particles into space-periodic systems that are sublattices of the considered crystal. The transformations of nonsymmorphic group transfers one sublattice into another, which is shifted on some translation $\alpha = (\alpha_1, \alpha_2, \alpha_3)$, $\alpha_i \in (0;1)$ (see the table of nonsymmorphic crystallographic groups in the appendix to the monograph [3]). Moreover, every particle in the new sublattice is turned by the corresponding transformation of the point group K .

At the crystallization phenomenon investigation naturally arises the problem of periodic solutions construction $u_i(q) = u_{0i} + w_i(q,\varepsilon)$, $w_j(q,\varepsilon) = \sum_{\mathbf{l}} w_{\mathbf{l}} e^{2\pi i \langle \mathbf{l}_j, q\rangle}$, ($\mathbf{l}_j = m_j^{(1)}\mathbf{l}^{(1)} + m_j^{(2)}\mathbf{l}^{(2)} + m_j^{(3)}\mathbf{l}^{(3)}$ is the inverse lattice vector) in the form of Fourier series on inverse lattice vectors, bifurcating from homogeneous density distribution $\rho_i(q) = \rho_{0i} = \frac{1}{v_{0i}}$, $v_{0j} = Mv_0$. Since the sublattices consist of identical but having different orientations particles and have the same translation group, we can take $\rho_{i0} = \rho_0$ and $u_{i0} = u_0$, and small parameter ε should be determined by the relation

$$\frac{\exp u_0}{Mv\theta\lambda} = \frac{\exp u_0}{Mv_0\theta_0\lambda_0} + \varepsilon = \mu_0 + \varepsilon.$$

System (2) in the vector-functions $w = \{w_i(q,\varepsilon)\}_1^M$ takes the form

$$B_s w_s \equiv w_s(q) + \mu_0 \sum_{j=1}^{M} \int K_{sj}(|q-q'|) w_j(q')dq' =$$
$$- \varepsilon \sum_{j=1}^{M} \int K_{sj}(|q-q'|) e^{w_j(q')} dq' - \mu_0 \sum_{j=1}^{M} \int K_{sj}(|q-q'|)[e^{w_j(q')} -$$
$$w_j(q') - 1]dq' \equiv R_s(w,\varepsilon) \quad (3)$$

Remark 2. By virtue of Remark 1, system (2) possesses the group symmetry of nonsymmorphic crystallographic group corresponding to the composite lattice consisting of M sublattices of one type molecules oriented by point group $K = C_{2h}$ ($|K| = M$, $|C_{2h}| = 4$) transformations. Nonsymmorphic group transformations transfer equations of the system (2) into each other, leaving invariant the whole system. The connection between the sublattices of the composite lattice and equations are realized by screw rotation and glide reflection.

The system of integral equations (3) is considered in the space of vector-functions $C^1(\Pi_0)$, Π_0 is the elementary cell of periodicity, and kernels $K_{sj}(|q-q'|)$ are sufficiently smooth, so $\int K_{sj}(|q-q'|)u_j(q')dq'$, $q \in \Pi_0$ can be differentiated with respect to the parameter q.

Further the general case of composite lattice will be illustrated by the example of crystallization with translation lattice consisting of four primitive sublattices Γ_m of monoclinic syngony with nonsymmorphic group C_{2h}^5 [3] which have nontrivial screw rotation and glide reflection.

Describe the zero-subspace of linearized system (3)

$$B_s w_s \equiv w_s(q) + \mu_0 \sum_{j=1}^{M} \int K_{sj}(|q-q'|) w_j(q')dq' = 0, \quad s = 1,\ldots,M \qquad (4)$$

presenting the components of vector-function w by Fourier series on inverse lattice vectors (index k is numbering the three-tuples of integers $(m_j^{(1)}, m_j^{(2)}, m_j^{(3)})$)

$$w_j(q') = \sum_k w_{kj} e^{2\pi i \langle \mathbf{l}_{kj}, q\rangle}, \quad \mathbf{l}_{kj} = m_{kj}^{(1)}\mathbf{l}^{(1)} + m_{kj}^{(2)}\mathbf{l}^{(2)} + m_{kj}^{(3)}\mathbf{l}^{(3)}, \quad m_{kj}^{(p)} \in \mathbb{Z}$$

$$B_s w_s = \sum_k w_{ks} e^{2\pi i \langle \mathbf{l}_{ks}, q\rangle} + \mu_0 \sum_{j=1}^{M} \int K_{sj}(|q-q'|) \sum_k w_{kj} e^{2\pi i \langle \mathbf{l}_{kj}, q'\rangle} dq' =$$

$$\sum_k w_{ks} e^{2\pi i \langle \mathbf{l}_{ks}, q\rangle} + \mu_0 \sum_{j=1}^{M} \int K_{sj}(|q-q'|) \sum_k w_{kj} e^{2\pi i \langle \mathbf{l}_{kj}, q\rangle} e^{-2\pi i \langle \mathbf{l}_{kj}, q-q'\rangle} dq' =$$

$$\sum_k w_{ks} e^{2\pi i \langle \mathbf{l}_{ks}, q\rangle} + \mu_0 \sum_k \sum_{j=1}^{M} w_{kj} e^{2\pi i \langle \mathbf{l}_{kj}, q\rangle} \int K_{sj}(|q-q'|) e^{-2\pi i \langle \mathbf{l}_{kj}, q-q'\rangle} dq' \tag{5}$$

Compute the integrals $I_{ts} = \int K_{ts}(|q-q'|) e^{-2\pi i \langle \mathbf{l}_{ks}, q-q'\rangle} dq'$. Setting $\tilde{q} = q - q' = x\mathbf{e}_1 + y\mathbf{e}_2 + z\mathbf{e}_3 = \tilde{x}\mathbf{a}_1 + \tilde{y}\mathbf{a}_2 + \tilde{z}\mathbf{a}_3$; $\mathbf{a}_j = a_{1j}\mathbf{e}_1 + a_{2j}\mathbf{e}_2 + a_{3j}\mathbf{e}_3$

$$\begin{pmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \mathbf{a}_3 \end{pmatrix} = A^T \begin{pmatrix} \mathbf{e}_1 \\ \mathbf{e}_2 \\ \mathbf{e}_3 \end{pmatrix} \Rightarrow \begin{pmatrix} x \\ y \\ z \end{pmatrix} = A \begin{pmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \end{pmatrix}$$

performing the change of variables

$$\begin{aligned} x &= \tilde{x}a_{11} + \tilde{y}a_{12} + \tilde{z}a_{13} \\ y &= \tilde{x}a_{21} + \tilde{y}a_{22} + \tilde{z}a_{23} \\ z &= \tilde{x}a_{31} + \tilde{y}a_{32} + \tilde{z}a_{33} \end{aligned}$$

and then carrying out the transition to spherical coordinates one get

$$I_{ts} = \int_0^\infty \rho^2 K(\rho) 2\pi \int_{-1}^{1} \exp\left[-\frac{2\pi i \rho}{det\ A} R_{ks} t\right] dt = \frac{2 det\ A}{R_{ks}} \int_0^\infty \rho K(\rho) \sin\left(\frac{2\pi \rho R_{ks}}{det\ A}\right) d\rho$$

Omitting tedious computations, write the expression for R_{ks}

$$R_{ks} = R(m_{ks}^{(1)}, m_{ks}^{(2)}, m_{ks}^{(3)}) =$$
$$\Big\{ {m_{ks}^{(1)}}^2 \left[(a_{21}^2+a_{22}^2+a_{23}^2)(a_{31}^2+a_{32}^2+a_{33}^2) - (a_{21}a_{31}+a_{22}a_{32}+a_{23}a_{33})^2\right] +$$
$${m_{ks}^{(2)}}^2 \left[(a_{11}^2+a_{12}^2+a_{13}^2)(a_{31}^2+a_{32}^2+a_{33}^2) - (a_{11}a_{31}+a_{12}a_{32}+a_{13}a_{33})^2\right] +$$
$${m_{ks}^{(3)}}^2 \left[(a_{21}^2+a_{22}^2+a_{23}^2)(a_{11}^2+a_{12}^2+a_{13}^2) - (a_{11}a_{21}+a_{12}a_{22}+a_{13}a_{23})^2\right] +$$
$$2m_{ks}^{(1)}m_{ks}^{(2)} \left[(a_{11}a_{31}+a_{12}a_{32}+a_{13}a_{33})(a_{21}a_{31}+a_{22}a_{32}+a_{23}a_{33}) - (a_{11}a_{21}+a_{12}a_{22}+a_{13}a_{23})(a_{31}^2+a_{32}^2+a_{33}^2)\right] +$$
$$2m_{ks}^{(1)}m_{ks}^{(3)} \left[(a_{11}a_{21}+a_{12}a_{22}+a_{13}a_{23})(a_{21}a_{31}+a_{22}a_{32}+a_{23}a_{33}) - (a_{11}a_{31}+a_{12}a_{32}+a_{13}a_{33})(a_{21}^2+a_{22}^2+a_{23}^2)\right] +$$
$$2m_{ks}^{(2)}m_{ks}^{(3)} \left[(a_{11}a_{21}+a_{12}a_{22}+a_{13}a_{23})(a_{11}a_{31}+a_{12}a_{32}+a_{13}a_{33}) - (a_{21}a_{31}+a_{22}a_{32}+a_{23}a_{33})(a_{11}^2+a_{12}^2+a_{13}^2)\right] \Big\}^{\frac{1}{2}} \tag{6}$$

System (5) takes the form

$$\sum_k w_{ks} e^{2\pi i (m_{ks}^{(1)}x + m_{ks}^{(2)}y + m_{ks}^{(3)}z)} -$$
$$\mu_0 \sum_k \sum_{j=1}^{M} w_{kj} e^{2\pi i (m_{kj}^{(1)}x + m_{kj}^{(2)}y + m_{kj}^{(3)}z)} \frac{2det\,A}{R_{kj}} \int_0^\infty \rho K_{sj}(\rho) \sin\left(\frac{2\pi\rho R_{kj}}{det\,A}\right) d\rho = 0 \tag{7}$$

with the determinant

$$\Delta_k = \left[I\delta_{sj} - \mu_0 \frac{2det\,A}{R_{kj}(m_{kj})} \int_0^\infty \rho K_{sj}(\rho) \sin\left(\frac{2\pi\rho R_{kj}(m_{kj})}{det\,A}\right) d\rho \right],\ s,j = \overline{1,M} \tag{8}$$

Thus, conversion to zero of the determinant (8) defines the eigenvalues μ_0 and presents the crystallization criterion [4] with corresponding composite lattice.

Kernels $K_{sj}(|q-q'|) = K_{js}(|q-q'|)$ are invariant with respect to the group of Euclidean space motion $\mathbb{R}^3$ including also the transformations g of non-symmorphic crystallographic groups G $K_{sj}(|gq-gq'|) = K_{sj}(|q-q'|)$. The corresponding operators $K_{sj}f(q) = \int K_{sj}(|q-q'|)f(q')dq'$ are invariant to the shift operators by virtue of kernels K_{sj} invariance relative to simultaneous motions in $\mathbb{R}^3$ of arguments q and q'. Indeed, since dq' is invariant relative to the G measure in $\mathbb{R}^3$, one has

$$(K_{sj}f)(gq) = \int K_{sj}(|gq-q'|)f(q')dq' \overset{q'=g\bar{q}}{=} \int K_{sj}(|q-\bar{q}|)f(g\bar{q})d\bar{q} = K_{sj}T(g)f(q)$$

Therefore, by applying nonsymmorphic transformation $T(g)$ to the s-th equation (4) one gets

$$T(g)w_s(q) + \mu_0 \sum_{j=1}^{M} \int K_{sj}(|q-\bar{q}|)w_j(g\bar{q})d\bar{q} =$$
$$= T(g)w_s(q) + \mu_0 \sum_{j=1}^{M} \int K_{sj}(|q-\bar{q}|)T(g)w_j(\bar{q})d\bar{q} = 0$$

Hence, together with some solution $w = (w_1, \ldots, w_M)^T$ of the linearized system (4) it has the solutions $T(g)w = (T(g)w_1, \ldots, T(g)w_M)^T$. Therefore system (4) is invariant to the transformations $T(g)$.

Further the obtained result is illustrated on the example of the nonsymmorphic group C_{2h}^5 of monoclinic syngony [3]. Here the basic translation vectors should be chosen in the form

$$\mathbf{a}_1 = \alpha\mathbf{i}, \quad \mathbf{a}_2 = \beta\mathbf{i} + \gamma\mathbf{j}, \quad \mathbf{a}_3 = \delta\mathbf{k}$$

such that the inverse lattice vectors take the form

$$\mathbf{l}^{(1)} = \frac{[\mathbf{a}_2, \mathbf{a}_3]}{\Omega} = \frac{1}{\alpha}\mathbf{i} - \frac{\beta}{\alpha\gamma}\mathbf{j}; \quad \mathbf{l}^{(2)} = \frac{[\mathbf{a}_3, \mathbf{a}_1]}{\Omega} = \frac{1}{\gamma}\mathbf{j}; \quad \mathbf{l}^{(3)} = \frac{[\mathbf{a}_1, \mathbf{a}_2]}{\Omega} = \frac{1}{\delta}\mathbf{k},$$

where $\Omega = \langle \mathbf{a}_1, [\mathbf{a}_2, \mathbf{a}_3] \rangle = \alpha\gamma\delta$.

$$R_{kj}^2 = \delta^2[m_{kj}^{(1)}\beta - m_{kj}^{(2)}\alpha]^2 + m_{kj}^{(1)^2}\gamma^2\delta^2 + m_{kj}^{(3)^2}\alpha^2\gamma^2$$

The group C_{2h}^5 is generated by the elements [3]

$(\frac{1}{2}t_z, r)$, $(\frac{1}{2}t_x, \sigma_h)$ and $(\frac{1}{2}t_x + \frac{1}{2}t_z, \sigma_h r)$. Then the functions $w_1 = e^{2\pi i\langle \mathbf{l}_1, q\rangle} = e^{2\pi i(m_{k1}^{(1)}\tilde{x} + m_{k1}^{(2)}\tilde{y} + m_{k1}^{(3)}\tilde{z})}$, $(\frac{1}{2}t_x + \frac{1}{2}t_z, \sigma_h r)w_1 = (-1)^{m_{k1}^{(1)} + m_{k1}^{(3)}} e^{2\pi i(-m_{k1}^{(1)}\tilde{x} - m_{k1}^{(2)}\tilde{y} - m_{k1}^{(3)}\tilde{z})}$, $(\frac{1}{2}t_x, \sigma_h)w_1 = (-1)^{m_{k1}^{(1)}} e^{2\pi i(m_{k1}^{(1)}\tilde{x} + m_{k1}^{(2)}\tilde{y} - m_{k1}^{(3)}z)}$, $(\frac{1}{2}t_z, r)w_1 = (-1)^{m_{k1}^{(3)}} e^{2\pi i(-m_{k1}^{(1)}\tilde{x} - m_{k1}^{(2)}\tilde{y} + m_{k1}^{(3)}\tilde{z})}$ are the first components of the vector solutions of linearized system (4).

Thus, according to Remark 2, the zero subspace is generated by the vector-functions $W = (w_1(q), \ldots, w_M(q))^T, T(g_1)W, \ldots, T(g_M)W$, $w_k(q) = T(g_k)w_1(q) = w_1(g_k q)$, $k = 1, \ldots, M$, where g_k are numbered together with sublattices elements of nonsymmorphic group symmetry. Since $T(g_k)$ can be stationary subgroup element, the dimension of the zero subspace of the linearized matrix operator $\mathbf{B} = \mathbf{B}(\mu_0) = (I - \mu_0 \mathcal{K})$ of the system (3), i.e. the multiplicity of the eigenvalue μ_0, may be equal to the divisors of the corresponding point group symmetry order or some of their sums in the case of several generating elements in the zero subspace $N(\mathcal{B})$ under the action of $g_k \in G$, $k = 1, \ldots, M$.

By virtue of the symmetry $K_{sj} = K_{js}$ the linearized matrix operator is symmetric and it generates a symmetric determinant of the system of algebraic equations.

Remark 3. The values R_{kj}, $j = 1, \ldots, M$ are invariant to the point group transformations. The proof of this assertion does not follow from symmetry considerations and it is checked for each nonsymmorphic group apart.

Four dimensional branching equation construction for the system (3) with group symmetry C_{2h}^5 of monoclinic syngony in the case of one general position vector generating $N(B)$

The connection between the sublattices of composite lattice and equations is realized by the transformations of the nonsymmorphic group

$$(\frac{1}{2}t_z, r) \cong (1,4)(2,3), \quad (\frac{1}{2}t_x, \sigma_h) \cong (1,3)(2,4), \quad (\frac{1}{2}t_x + \frac{1}{2}t_z, \sigma_h r) \cong (1,2)(3,4) \tag{9}$$

The equations transferring into each other it is necessary to fulfill the following symmetry relations between the kernels of the integral operators

$$\begin{array}{ll} K_{11} = \ldots = K_{44}; & K_{14} = K_{23} = K_{32} = K_{41}; \\ K_{12} = K_{21} = K_{34} = K_{43}; & K_{13} = K_{31} = K_{24} = K_{42}. \end{array} \tag{10}$$

It is practically impossible to perform bifurcating equation construction in the case of arbitrary $m_{k1}^{(j)}$, thus for the simplicity take $m_{k1}^{(j)} = 1$.

Choose the basis vectors of the zero subspace $N(\mathbf{B})$ in the form

$$\Phi_1 = \begin{pmatrix} \varphi_1 & = & e^{2\pi i(x+y+z)} \\ \varphi_2 & = & e^{2\pi i(-x-y-z)} \\ \varphi_3 & = & -e^{2\pi i(x+y-z)} \\ \varphi_4 & = & -e^{2\pi i(-x-y+z)} \end{pmatrix}, \quad \Phi_2 = (\tfrac{1}{2}t_x + \tfrac{1}{2}t_z, \sigma_h r)\Phi_1 = \begin{pmatrix} \varphi_2 \\ \varphi_1 \\ \varphi_4 \\ \varphi_3 \end{pmatrix},$$

$$\Phi_3 = (\tfrac{1}{2}t_x, \sigma_h)\Phi_1 = \begin{pmatrix} \varphi_3 \\ \varphi_4 \\ \varphi_1 \\ \varphi_2 \end{pmatrix}, \qquad \Phi_4 = (\tfrac{1}{2}t_z, r)\Phi_1 = \begin{pmatrix} \varphi_4 \\ \varphi_3 \\ \varphi_2 \\ \varphi_1 \end{pmatrix}$$

For the simplification of notations hereinafter we will omit the symbol "tilde", i.e. x, y, z will be considered as coordinates along axes $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$ respectively.

In order to compute the bifurcating solutions in the neighborhoods of the parameter critical value, bifurcation theory methods [5] are applied.

Let E_1 and E_2 be two Banach spaces. The nonlinear equation

$$Bx = R(x, \lambda), \quad R(0,0) = 0, \ R_x(0,0) = 0 \tag{11}$$

is considered. Here $B : E_1 \to E_2$ is a closed linear Fredholm operator ($R(B) = \overline{R(B)}$, $R(B)$ is the range of the operator B) with dense in E_1 domain $D(B)$, $N(B) = \mathrm{span}\{\Phi_1, \ldots, \Phi_n\}$ is its null-subspace, $N^*(B) = \mathrm{span}\{\Psi_1, \ldots, \Psi_n\} \subset E_2^*$ is its defect-subspace. The nonlinear operator $R(x, \lambda)$ is supposed to be defined and sufficiently smooth in x and λ in a neighborhood of $(0,0) \in E_1 \dot{+} \Lambda$, Λ is the parameter space. According to Hahn-Banach theorem there exist biorthogonal systems $\{\Gamma_j\}_1^n \in E_1$, $\langle \Phi_i, \Gamma_j \rangle = \delta_{ij}$ and $\{Z_k\}_1^n \in E_2$, $\langle Z_k, \Psi_l \rangle = \delta_{kl}$, generating the projectors $P = \sum\limits_{j=1}^{n} \langle \cdot, \Gamma_j \rangle \varphi_j : E_1 \to N(B)$, $Q = \sum\limits_{j=1}^{n} \langle \cdot, \Psi_j \rangle z_j : E_2 \to E_{2,n} = \mathrm{span}\{z_1, \ldots, z_n\}$ and the following direct sum expansions $E_1 = E_1^n \dot{+} E_1^{\infty-n}$, $E_1^n = N(B)$, $E_2 = E_{2,n} \dot{+} E_{2,\infty-n}$, $E_{2,\infty-n} = R(B)$. Then the Lyapounov-Schmidt method allows to reduce the problem (11) of construction of small norm solutions to nonlinear finite-dimensional equations system that is the bifurcation equation.

Here $Z_s = \Phi_s$,

$$\Gamma_1 = \Psi_1 = \frac{1}{4|\Pi_0|}\Phi_2,\ \Gamma_2 = \Psi_2 = \frac{1}{4|\Pi_0|}\Phi_1,\ \Gamma_3 = \Psi_3 = \frac{1}{4|\Pi_0|}\Phi_4,\ \Gamma_4 = \Psi_4 = \frac{1}{4|\Pi_0|}\Phi_3$$

Write system (3) in the power series expansion introducing the parameters ξ_k, $k = 1, \ldots, 4$ and the Schmidt correction operator

$$\begin{aligned}
\tilde{B}W &= \begin{pmatrix} w_1(q) \\ \cdots \\ w_4(q) \end{pmatrix} + \mu_0 \mathcal{K} W + \sum_{j=1}^{4} \langle W, \Gamma_j \rangle Z_j = -\varepsilon \begin{pmatrix} \sum_{j=1}^4 K_{1j}(|q-q'|)dq' \\ \cdots \\ \sum_{j=1}^4 K_{4j}(|q-q'|)dq' \end{pmatrix} \qquad (11) \\
&\quad -\varepsilon \mathcal{K} \begin{pmatrix} w_1(q') + \frac{w_1(q')^2}{2!} + \ldots \\ \cdots \\ w_4(q') + \frac{w_4(q')^2}{2!} + \ldots \end{pmatrix} - \mu_0 \mathcal{K} \begin{pmatrix} \frac{w_1(q')^2}{2!} + \frac{w_1(q')^3}{3!} + \ldots \\ \cdots \\ \frac{w_4(q')^2}{2!} + \frac{w_4(q')^3}{3!} + \ldots \end{pmatrix} + \sum_{j=1}^{4} \xi_j Z_j \\
\xi_j &= \langle W, \Gamma_j \rangle
\end{aligned}$$

$$\mathcal{K} = \begin{pmatrix} \int K_{11}(q')dq' & \ldots & \int K_{14}(q')dq' \\ \cdots & \cdots & \cdots \\ \int K_{41}(q')dq' & \ldots & \int K_{44}(q')dq' \end{pmatrix}$$

By the implicit operators theorem the first equation (12) has a unique solution $W = W(\xi, \varepsilon)$. Branching system takes the form

$$L^{(i)}(\xi, \varepsilon) \equiv \xi_i - \langle W(\xi, \varepsilon), \Gamma_i \rangle = 0, \quad i = 1, \ldots, 4$$

We find the solutions of the first equation (12) in the form of the series $W(q, \varepsilon) = \sum\limits_{|\alpha|+k \geq 1} W_{\alpha;k} \xi^\alpha \varepsilon^k$.

Omitting tedious computations write out the main part of the branching system

$$\begin{aligned}
f_1(\xi, \varepsilon) &= A\xi_1\varepsilon + B{\xi_2}^3 + C{\xi_1}^2\xi_2 + D\xi_1\xi_3\xi_4 + E\xi_2{\xi_3}^2 + F\xi_2{\xi_4}^2 + \ldots = 0 \qquad (12) \\
f_2(\xi, \varepsilon) &= A\xi_2\varepsilon + B{\xi_1}^3 + C{\xi_2}^2\xi_1 + D\xi_2\xi_3\xi_4 + E\xi_1{\xi_4}^2 + F\xi_1{\xi_3}^2 + \ldots = 0 \\
f_3(\xi, \varepsilon) &= A\xi_3\varepsilon + B{\xi_4}^3 + C{\xi_3}^2\xi_4 + D\xi_1\xi_2\xi_3 + E\xi_4{\xi_1}^2 + F\xi_4{\xi_2}^2 + \ldots = 0 \\
f_4(\xi, \varepsilon) &= A\xi_4\varepsilon + B{\xi_3}^3 + C{\xi_4}^2\xi_3 + D\xi_1\xi_2\xi_4 + E\xi_3{\xi_2}^2 + F\xi_3{\xi_1}^2 + \ldots = 0
\end{aligned}$$

The obtained system allows the group (9) of substitutions $p_1 = (12)(34)$, $p_2 = (13)(24)$, $p_3 = (13)(23)$.

Passing to real variables $\xi_1 = \tau_1 + i\tau_2$, $\xi_2 = \tau_1 - i\tau_2$, $\xi_3 = \tau_3 + i\tau_4$, $\xi_4 = \tau_3 - i\tau_4$ one gets the branching system in the new base

$$\widehat{\Phi}_1 = \begin{pmatrix} \cos 2\pi(x+y+z) \\ \cos 2\pi(x+y+z) \\ -\cos 2\pi(x+y-z) \\ -\cos 2\pi(x+y-z) \end{pmatrix}, \quad \widehat{\Phi}_2 = \begin{pmatrix} \sin 2\pi(x+y+z) \\ -\sin 2\pi(x+y+z) \\ -\sin 2\pi(x+y-z) \\ \sin 2\pi(x+y-z) \end{pmatrix},$$

$$\widehat{\Phi}_3 = \begin{pmatrix} -\cos 2\pi(x+y-z) \\ -\cos 2\pi(x+y-z) \\ \cos 2\pi(x+y+z) \\ \cos 2\pi(x+y+z) \end{pmatrix}, \quad \widehat{\Phi}_4 = \begin{pmatrix} -\sin 2\pi(x+y-z) \\ \sin 2\pi(x+y-z) \\ \sin 2\pi(x+y+z) \\ -\sin 2\pi(x+y+z) \end{pmatrix}.$$

$$\begin{aligned}
t_1(\tau,\varepsilon) &= A\tau_1\varepsilon + B\tau_1(\tau_1^2 - 3\tau_2^2) + C\tau_1(\tau_1^2+\tau_2^2) + D\tau_1(\tau_3^2+\tau_4^2) + \\
&\quad + E[\tau_1(\tau_3^2-\tau_4^2) + 2\tau_2\tau_3\tau_4] + F[\tau_1(\tau_3^2-\tau_4^2) - 2\tau_2\tau_3\tau_4] + \ldots = 0 \qquad (13)\\
t_2(\tau,\varepsilon) &= A\tau_2\varepsilon + B\tau_2(\tau_2^2 - 3\tau_1^2) + C\tau_2(\tau_1^2+\tau_2^2) + D\tau_2(\tau_3^2+\tau_4^2) + \\
&\quad + E[-\tau_2(\tau_3^2-\tau_4^2) + 2\tau_1\tau_3\tau_4] - F[\tau_2(\tau_3^2-\tau_4^2) + 2\tau_1\tau_2\tau_4] + \ldots = 0\\
t_3(\tau,\varepsilon) &= A\tau_3\varepsilon + B\tau_3(\tau_3^2 - 3\tau_2^2) + C\tau_3(\tau_3^2+\tau_4^2) + D\tau_3(\tau_1^2+\tau_2^2) + \\
&\quad + E[\tau_3(\tau_1^2-\tau_2^2) + 2\tau_1\tau_2\tau_4] + F[\tau_3(\tau_1^2-\tau_2^2) - 2\tau_1\tau_2\tau_4] + \ldots = 0\\
t_4(\tau,\varepsilon) &= A\tau_4\varepsilon + B\tau_4(\tau_4^2 - 3\tau_3^2) + C\tau_4(\tau_3^2+\tau_4^2) + D\tau_4(\tau_1^2+\tau_2^2) + \\
&\quad + E[-\tau_4(\tau_1^2-\tau_2^2) + 2\tau_1\tau_2\tau_3] - F[\tau_4(\tau_1^2-\tau_2^2) + 2\tau_1\tau_2\tau_3] + \ldots = 0
\end{aligned}$$

Applying the transformations

$$\begin{aligned}
t_1\tau_2 - t_2\tau_1 &= 2B\tau_1\tau_2(\tau_1^2-\tau_2^2) + E[\tau_1\tau_2(\tau_3^2-\tau_4^2) - \tau_3\tau_4(\tau_1^2-\tau_2^2)] + \\
&\quad +F[\tau_1\tau_2(\tau_3^2-\tau_4^2) + \tau_3\tau_4(\tau_1^2-\tau_2^2)] + \ldots = 0 \\
t_1\tau_2 + t_2\tau_1 &= A\tau_1\tau_2\varepsilon + (C-2B)\tau_1\tau_2(\tau_1^2+\tau_2^2) + D\tau_1\tau_2(\tau_3^2+\tau_4^2) + \\
&\quad +(E-F)\tau_3\tau_4(\tau_1^2+\tau_2^2) + \ldots = 0 \\
t_3\tau_4 - t_4\tau_3 &= 2B\tau_3\tau_4(\tau_3^2-\tau_4^2) + E[\tau_3\tau_4(\tau_1^2-\tau_2^2) - \tau_1\tau_2(\tau_3^2-\tau_4^2)] + \\
&\quad +F[\tau_3\tau_4(\tau_1^2-\tau_2^2) + \tau_1\tau_2(\tau_3^2-\tau_4^2)] + \ldots = 0 \\
t_3\tau_4 + t_4\tau_3 &= A\tau_3\tau_4\varepsilon + (C-2B)\tau_3\tau_4(\tau_3^2+\tau_4^2) + D\tau_3\tau_4(\tau_1^2+\tau_2^2) + \\
&\quad +(E-F)\tau_1\tau_2(\tau_3^2+\tau_4^2) + \ldots = 0
\end{aligned} \tag{14}$$

adding and subtracting first and third, second and fourth equation of the system (15) bring the branching system to the form

$$\begin{aligned}
\tilde{t}_1(\tau,\varepsilon) &= B[\tau_1\tau_2(\tau_1^2-\tau_2^2) + \tau_3\tau_4(\tau_3^2-\tau_4^2)] + \\
&\quad +F[\tau_1\tau_2(\tau_3^2-\tau_4^2) + \tau_3\tau_4(\tau_1^2-\tau_2^2)] + \ldots = 0 \\
\tilde{t}_2(\tau,\varepsilon) &= B[\tau_1\tau_2(\tau_1^2-\tau_2^2) - \tau_3\tau_4(\tau_3^2-\tau_4^2)] + \\
&\quad +E[\tau_1\tau_2(\tau_3^2-\tau_4^2) - \tau_3\tau_4(\tau_1^2-\tau_2^2)] + \ldots = 0 \\
\tilde{t}_3(\tau,\varepsilon) &= A\varepsilon(\tau_1\tau_2+\tau_3\tau_4) + (C-B)[\tau_1\tau_2(\tau_1^2+\tau_2^2) + \tau_3\tau_4(\tau_3^2+\tau_4^2)] + \\
&\quad +(D+E-F)[\tau_1\tau_2(\tau_3^2+\tau_4^2) + \tau_3\tau_4(\tau_1^2) + \tau_2^2] + \ldots = 0 \\
\tilde{t}_4(\tau,\varepsilon) &= A\varepsilon(\tau_1\tau_2-\tau_3\tau_4) + (C-B)[\tau_1\tau_2(\tau_1^2+\tau_2^2) - \tau_3\tau_4(\tau_3^2+\tau_4^2)] + \\
&\quad +(D-E+F)[\tau_1\tau_2(\tau_3^2+\tau_4^2) - \tau_3\tau_4(\tau_1^2) + \tau_2^2] + \ldots = 0
\end{aligned} \tag{15}$$

Note that the written system in the real basis possesses the substitutions

$$\begin{gathered}
p_1: \tau_1 \to \tau_1,\ \tau_2 \to -\tau_2,\ \tau_3 \to \tau_3,\ \tau_4 \to -\tau_4; \\
p_2: \tau_1 \leftrightarrow \tau_3,\ \tau_2 \leftrightarrow \tau_4; \quad p_3: \tau_1 \leftrightarrow \tau_3,\ \tau_2 \leftrightarrow -\tau_4
\end{gathered} \tag{17}$$

The first two equations (16) are considered as the system relative to $(\tau_1^2-\tau_2^2)$, $(\tau_3^2-\tau_4^2)$ with determinant $\Delta = 2[\tau_1\tau_2\tau_3\tau_4(EF-B^2)+B(E-F)(\tau_1^2\tau_2^2+\tau_3^2\tau_4^2)]$.

I. If $\Delta \neq 0$, which is possible for $(B^2-EF)^2-4B^2(E-F)^2<0$ ($|B^2-EF| < 2|B(E-F)|$), then $\tau_1^2=\tau_2^2\neq 0$ and $\tau_3^2=\tau_4^2\neq 0$ (inequality to zero should be taken place at least in one case). Then the last two equations of the system (16) are reducing to one of the following forms

A. $\tau_1=\tau_2$, $\tau_3=\tau_4$.

For $\tau_1\neq 0$, $\tau_3\neq 0$ one has

$$A\varepsilon+2(C-B)\tau_1^2+2(D+E-F)\tau_3^2=0$$
$$A\varepsilon+2(C-B)\tau_3^2+2(D+E-F)\tau_1^2=0$$

$\tau_1=\pm\tau_3=\pm\sqrt{\frac{-A\varepsilon}{2(-B+C-D-E+F)}}+o(|\varepsilon|^{1/2})$, $sign\,\varepsilon=-sign\,A(-B+C-D-E+F)$, any sign combinations are possible

For $\tau_1\neq 0$, $\tau_3=0$ one gets the equation $A\tau_1^2\varepsilon-2B\tau_1^4=0$

$$\tau_1=\pm\sqrt{\frac{A\varepsilon}{2B}}+o(|\varepsilon|^{1/2}),\quad sign\,\varepsilon=sign\,(AB)$$

For $\tau_1=0$, $\tau_3\neq 0$ one gets $A\tau_3^2\varepsilon-2B\tau_3^4=0$

$$\tau_3=\pm\sqrt{\frac{A\varepsilon}{2B}}+o(|\varepsilon|^{1/2}),\quad sign\,\varepsilon=sign\,(AB)$$

In the case **B.** $\tau_1=-\tau_2$, $\tau_3=-\tau_4$ we obtain the same equations.

C. $\tau_1=-\tau_2$, $\tau_3=\tau_4$.

For $\tau_1\neq 0$ č $\tau_3\neq 0$ one has

$$A\varepsilon+2(-B+C)\tau_1^2+2(D-E+F)\tau_3^2=0$$
$$-A\varepsilon+2(B-C)\tau_3^2+2(-D+E-F)\tau_1^2=0$$

$$\tau_1=\pm\sqrt{\frac{-A\varepsilon}{2(-B+C+D-E+F)}}+o(|\varepsilon|^{1/2}),$$
$$sign\,\varepsilon=-sing\,A(-B+C+D-E+F);$$
$$\tau_3=\pm\sqrt{\frac{A\varepsilon}{2(B-C+D-E+F)}}+o(|\varepsilon|^{1/2}),$$
$$sign\,\varepsilon=sing\,A(B-C+D-E+F)$$

For $\tau_1 \neq 0$, $\tau_3 = 0$ one gets the equation $A\varepsilon + 2(-B+C)\tau_1^2 = 0$

$$\tau_1 = \pm\sqrt{\frac{A\varepsilon}{2(B-C)}} + o(|\varepsilon|^{1/2}), \quad sign\,\varepsilon = sign\,A(B-C)$$

For $\tau_1 = 0$, $\tau_3 \neq 0$ one gets $-A\varepsilon + 2(B-C)\tau_3^2 = 0$

$$\tau_3 = \pm\sqrt{\frac{A\varepsilon}{2(B-C)}} + o(|\varepsilon|^{1/2}), \quad sign\,\varepsilon = sign\,A(B-C)$$

In the case **D.** $\tau_1 = -\tau_2$, $\tau_3 = \tau_4$ we obtain the same equations.

II. Let $\Delta = 0$, which is possible for $(B^2-EF)^2 \geq 4B^2(E-F)^2$ ($|B^2-EF| \geq 2|B(E-F)|$), then if $E \neq F$

$$\tau_3\tau_4 = \frac{B^2 - EF \pm \sqrt{(B^2-EF)^2 - 4B^2(E-F)^2}}{2B(E-F)}\tau_1\tau_2 = k\tau_1\tau_2.$$

Then the last two equations of the system (16) are written in the form

$$(\tau_1^2+\tau_2^2)[(C-B)+k(E-F)] + (\tau_3^2+\tau_4^2)D = -A\varepsilon,$$
$$(\tau_1^2+\tau_2^2)k + (\tau_3^2+\tau_4^2)[(C-B)+k(E-F)] = -Ak\varepsilon,$$

whence

$$\tau_1^2+\tau_2^2 = \frac{-A\varepsilon[(C-B)+k(E-F)-D]}{[(C-B)+k(E-F)]^2-kD},$$
$$\tau_3^2+\tau_4^2 = \frac{-A\varepsilon[(C-B)+k(E-F)-1]}{[(C-B)+k(E-F)]^2-kD}.$$

Thus, all obtained solutions are presented in the form of series, converging in the small neigbourhood of $\varepsilon = 0$, $W = \sum \tau_k^0(\varepsilon^{1/2})\widehat{\Phi}_k + O(|\varepsilon|)$, where $\tau_k^0(\varepsilon^{1/2})$ are the leading terms. Taking into account group transformations their number can be decreased.

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