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HYPERFINE INTERACTIONS VERSUS INTRINSIC SYMMETRIES OF MANY-ELECTRON SYSTEMS IN NEAR-SURFACE REGIONS

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ABSTRACT. The paper aims at unifying various types of hyperfine interactions from the viewpoint of Finsler geometry and supercomplex structures, reflecting the intrinsic symmetries of many-electron systems, with special reference to near-surface regions.

INTRODUCTION

The paper is an extended version of [1, 2] with special attention paid to near-surface regions.

The core of the subject are *hyperfine interactions*. They seem to be quite important and not yet satisfactorily developed as far as many-particle systems are concerned. They include, in fact, various types of couplings between electromagnetic and other interactions, all of them of the third and fourth orders with respect to the annihilation and creation operators.

In the present paper a unification of the hyperfine interactions is proposed from the viewpoint of Finsler geometry and supercomplex structures [3, 4], reflecting the *intrinsic symmetries* of the system. The unification is proceeded by a separate discussion of hyperfine interactions for paramagnets in connection with the generalised Langevin equation, for ferromagnets in connection with Oguchi's theorem, and for ferroelectrics in connection with solitary waves.

The intrinsic symmetries of a many-electron system give rise to the construction of a suitable supercomplex structure and the corresponding hamiltonian. Then it is possible to derive from the latter a kind of generalised Breit equations which can be interpreted as generalised Fueter equations generating holomorphic mappings in the hypercomplex analysis corresponding to the supercomplex structure in question. An explicit relationship is given between those mappings and the spinors involved in the generalised Breit equations. In this sense the paper is a natural continuation of [5, 6].

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The general procedure is then applied to the three particular cases of hyperfine couplings discussed before, including some examples which seem to show the usefulness of the procedure.

After the section on Langevin-type equations in supercomplex geometry, as an example, an application to paramagnetic binary alloys of the type A_xB_{1-x} is given, including calculations of the configurational entropy and the temperature dependence of the order parameters [7, 8].

The second quantization and Oguchi's theorem in supercomplex geometry give a theoretical proof of the dependence of the band structure on temperature with a possibility of numerical calculations and corrections to the electron correlation functions as well as explain the influence of the higher order correlation on the relaxation processes.

In connection with the third particular case concerned with ferroelectrics, it appears that the generalised Breit equations always generate a generalised Kadomtsev-Petviashvili system of equations having, in general, soliton solutions. The application to the vibrational properties of ferroelectrics includes an observation that the theory of vibrations of ultra-heavily doped semiconductor binary alloys of the type $G_{1-x}P_x$, containing electrically inactive ions P_1 and electrically active ions P_2, has its natural counterpart for ferroelectric crystals of the KDP, TGS, and related types [9–11].

In addition, the applicability of the general approach to Raman scattering is indicated, in particular in the case of near-surface regions.

The conclusions concentrate on an observation that the formulae obtained imply the occurrence of the dipole interactions which come from the spin orientations characterized in terms of supercomplex structures. In the case of a system of electrons, bounded by a surface, the flux of the electromagnetic field, manifesting itself as a deformation of the space outside the object, determines in a natural way the *demagnetizing fields* existing in the region over the surface. The occurrence of those fields, experimentally measurable, enables us to determine the boundary conditions for solutions describing the electron density distribution inside the system. That is to say that the boundary conditions can be expressed *via deformation of the metric* in near-surface regions.

1. HYPERFINE INTERACTION FOR PARAMAGNETIC AND THE GENERALISED LANGEVIN EQUATION

In the case of free paramagnetic atoms, an external magnetic field applied to their source introduces a certain *order* and the decoupling effects occur when the electronic precession frequencies exceed considerably the hyperfine frequency [12]. For paramagnetic crystals of the rare earths there, most probably, exists a kind of angular *correlation resonance* for certain values of an applied magnetic field which leads to crossings of hyperfine levels [13]. The time-dependent

hyperfine interaction appears when the paramagnetic relaxation time is sufficiently yet not too small. In the case of paramagnetic ions in liquids they seem to be connected with coupling the electric moments of the shell and rapidly fluctuating electric fields due to the Brownian motion. Other reasons are impacts and, consequently, direct displacements of atoms. In garnets, the hyperfine fields direction at the rare earth nuclei fluctuates even below the ferromagnetic Néel point [14, 15].

Omitting electromagnetic interactions in an *anharmonic* paramagnetic *crystal* we can consider it a system of coupled anharmonic oscillators with fluctuations of the crystallographic lattice. In that case we arrive at a *generalised* (inhomogeneous) *Langevin equation* [16, 17]

$$(d^2/dt^2)\langle \underline{q}(\underline{\delta}, t)\rangle = -\underline{A}(0)\langle \underline{q}(\underline{\delta}, t)\rangle + \underline{\mathscr{F}}(t), \tag{1}$$

where $\underline{q}(\underline{\delta}, t)$ denotes the thermal displacement at the instant t for an atom whose position and local fluctuations are described by the generalised co-ordinates $\underline{\delta}$, $\langle \underline{q}\rangle$ is the average value of $\underline{q}$ calculated in the usual way in terms of the Gaussian distribution, the matrix $\underline{A}(0)$ consists of the force constants [18, 19], and $\underline{\mathscr{F}}(t)$ is the stochastic force connected with the particle in question considered a Brownian particle embedded in the heat bath of the remaining particles. The description [15], which includes in fact only the phonon vibrations, leads to the effective formulae for the *autocorrelation* $\langle :q^j(\delta, t)q^k(\delta, t+\tau):\rangle_t$ and the corresponding momentum autocorrelation of the related quantum operators. The method can also be extended to the case of scattering by liquids when the correlations of the particle velocities play an essential role. The inclusion of the electronic vibrations and the electron-phonon coupling to the hamiltonian leads, in general, to *soliton solutions* [20].

In the case when an *adatom* (i.e. an atom on the crystal surface) is the particle in question, the Langevin equation has the same form (1), but the solutions are essentially different [21]. The reason is that an adatom has its neighbours only in the half-space restricted by the surface. It gives new expressions for $A(0)$ and $\mathscr{F}(t)$, and new boundary conditions.

2. HYPERFINE INTERACTION FOR FERROMAGNETS, AND OGUCHI'S THEOREM

In ferromagnets, internal fields cause very strong perturbations. The resulting perturbation can, on the average, be treated in the same manner as an isotropic hyperfine interaction provided that the source is completely unpolarized and the Weiss regions are small enough. An isotope with a known excited state magnetic moment can serve, like in *Mössbauer effect* measurements, as a probe for investigating magnetic fields at the position of the nucleus [14] (solutions of diamagnetic substances in iron and rare earth metals in iron garnets and ferrites).

More generally, angular *correlations* have features in common with the Mössbauer technique. Extending the method of [13] to the *electron spins* $S(\underline{\delta}, t)$, we arrive at Oguchi's theorem [22] stating that the third component S^z of S satisfies the equation

$$(\partial/\partial t)\langle S^z(\underline{\delta}, t)\rangle = -(1/T_1)[\langle S^z(\underline{\delta}, t)\rangle - \langle S^z(\underline{\delta}, t)\rangle_{\text{l.e.}}], \tag{2}$$

where T_1 denotes the spin-lattice relaxation time and l.e. stands for 'local equilibrium'.

Indeed, if in the considerations of [13] we replace formally

$$(\partial/\partial t)\langle \underline{q}(\underline{\delta}, t)\rangle \quad \text{by} \quad \langle S^z(\underline{\delta}, t)\rangle,$$

then the counterpart of

$$(\partial^2/\partial t^2)\langle \underline{q}(\underline{\delta}, t)\rangle \quad \text{becomes} \quad -(1/T_1)[\langle S^z(\underline{\delta}, t) - S^z(\underline{\delta}, t)\rangle_{\text{l.e.}}],$$

as required.

Oguchi's theorem implies the linear *dependence of the energy of the hyperfine interaction on* the values of the electron and nuclear *spins* [23]. For precise interrelations with the Mössbauer line shape in the case of diluted ferromagnetic alloy thin films we refer to [24].

3. HYPERFINE INTERACTION FOR FERROELECTRICS AND THE APPEARANCE OF SOLITARY WAVES

In analogy to the internal fields in ferromagnets it is natural to consider in a similar way the fields in ferroelectrics, especially the electric fields available to saturate the sample giving conditions similar to those in a single crystal (the isotopes $NaTaO_3$, $PbTiO_3$, $BaTiO_3$, WO_3, etc.). At present, in analogy to $BaTiO_3$, the so-called Perovskite structures are being studied in the Escuela Superior de Física y Matemáticas del Instituto Politecnico Nacional in Mexico [25].

Experimental data and fenomenological considerations [26, 27] show that in the case in question the counterpart of the equation (1) has *soliton solutions*. Even in the case of ferroelectric crystals presenting a molecular group (e.g. $NaNO_2$) and a rather simple microscopic model [26], a double sine-Gordon equation is obtained:

$$u_{xt} = \sin u - \gamma \sin 2u, \tag{3}$$

where γ is a real constant. One solution of (3) is stable and can be interpreted as a motion of a ferroelectric wall with electromechanical couplings.

The solutions in question express *surface solitons* if the maximum is attained on the surface of the crystal, i.e. at the end of the chain of atoms in the sense of the construction given in [17], pp. 48–49. On the basis of the continualized equations of the magnetoelasticity for ferromagnetic crystals, it is shown in [26] that Bloch walls in an infinite crystals and Néel walls in a thin elastic film can be represented by 'magnetoelastic' solitary waves.

4. THE FINSLER GEOMETRY

The *Finsler geometry* is a generalisation of the Riemannian geometry [28]. Namely, let M be a real C^∞-manifold of dimension n. Then, let $L : TM \to \mathbf{R}_+ \cup \{0\}$ be a positive-valued C^∞-function defined on the bundle tangent to M with the following properties: (i) $L(x, Y) > 0$ for every $x \in M$ and $Y \in T_x M$, $Y \neq 0$, where $T_x M$ denotes the space tangent to M at x, (ii) $L(x, kY) = kL(x, Y)$ for any positive number k and every $x \in M$ and $Y \in T_x M$, (iii) locally,

$$\det [(\partial^2/\partial Y^j \partial Y^m) L^2(x, Y)] \neq 0 \quad \text{for every } x \in M .$$

A manifold M with the function L is called a *Finsler manifold.*

Since L^2 is a homogeneous function of degree 2 with respect to Y, then

$$L^2(x, Y) = \sum_{j,m} g_{jm}(x, Y)\, Y^j Y^m ,$$

where

$$g_{jm}(x, Y) := \tfrac{1}{2}(\partial^2/\partial Y^j \partial Y^m) L^2(x, Y) \tag{4}$$

is called a *Finslerian metric tensor.* The Finsler geometry reduces to the Riemannian geometry whenever the metric (4) is independent of Y.

In Finsler mechanics we assume a particle interacting with the electromagnetic field to be described by the function

$$L(x, \dot{x}) = (\sum_{h,j} a_{hj} \dot{x}^h \dot{x}^j)^{1/2} + \sum_j A_j \dot{x}^j ,$$

where $[a_{hj}]$ is a positive definite matrix consisting of the C^∞-functions defined on M and A_j are arbitrary C^∞-functions on M. It is clear that, in contrast to Riemannian geometry, in the Finsler geometry all the solitons are solutions of the equations of motion, i.e. of the Euler-Lagrange equations [5, 20].

5. SUPERCOMPLEX STRUCTURES

We consider two finite-dimensional real vector spaces S and V, equipped with scalar products $(,)_S$ and $(,)_V$. Let $(a, b)_S \in \mathbf{R}$ (the real number field), $(b, a)_S = (a, b)_S$, $(\gamma a, b)_S = \gamma (a, b)_S$, and $(a, b+c)_S = (a, b)_S + (a, c)_S$ whenever $a, b, c \in S$ and $\gamma \in \mathbf{R}$. For $f, g \in V$, we suppose that $(g, f)_V = \delta (f, g)_V$, $\delta = 1$ or -1; the remaining postulates for $(,)_V$ are the same as for $(,)_S$. Without any loss of generality we can choose the basis (ε_α) of S so that

$$[\eta_{\alpha\beta}] := [(\varepsilon_\alpha, \varepsilon_\beta)_S] = \operatorname{diag}(\underbrace{1, \ldots, 1}_{p \text{ times}}, -1, \ldots, -1). \tag{5}$$

A *multiplication* of elements of S by elements of V is defined as a mapping $S \times V \to V$ such that, for $f, g \in V$ and $a, b \in S$, we have $(a+b)f = af + bf$, $\alpha(f+g) = \alpha f + \alpha g$,

$$(\alpha, \alpha)_S (f, g)_V = (\alpha f, \alpha g)_V . \quad \textit{(the generalised Hurwitz condition)}, \tag{6}$$

and for which there exists a unit element ε_0 in S with respect to the multiplication.

A particularly important case appears when the pair (V, S) is *irreducible*, i.e. when it is not reducible. It is said to be reducible if there are real vector subspaces V_1 and V_2 of $V, \emptyset \neq V_1 \neq V_2$, $V_1 \oplus V_2 = V$, such that the images of $S \times V_1$ and $S \times V_2$ under the multiplication are contained in V_1 and V_2, respectively. The irreducible pair (V, S) satisfying all the above conditions is called a (*pseudo-euclidean*) *Hurwitz pair* [29, 3, 4].

Any Hurwitz pair induces a Clifford algebra with generators $\gamma_\alpha, \alpha = 1, ..., p-1$, determined by the relations

$$C_\alpha = i\gamma_\alpha C_p, \quad C_a := [c^k_{ja}], \quad c^k_{ja} = (e^k, \varepsilon_a e_j)_V, \quad e^k := \varkappa^{ks} e_s,$$

where $a = 1, ..., p$; $j, k = 1, ..., n = \dim V$, i denotes the imaginary unit, and the Einstein summation convention is assumed. The generators are chosen in the imaginary *Majorana representation*: they are purely imaginary and satisfy conditions analogous to those fulfilled by the familiar Dirac matrices

$$\bar{\gamma}_\alpha = -\gamma_\alpha, \quad \operatorname{re}\gamma_\alpha = 0, \quad \gamma_\alpha\gamma_\beta + \gamma_\beta\gamma_\alpha = 2\hat{\eta}_{\alpha\beta} I_n, \quad \beta \neq \alpha,$$

$$\hat{\eta}_{\alpha\beta} := \eta_{\alpha\beta}/\eta_{pp}, \quad \eta_{pp} = 1 \quad \text{or} \quad -1,$$

where $[\eta_{\alpha\beta}]$ is defined in (5) and I_n denotes the identity $n \times n$-matrix.

Define S_α by $S_\alpha = -i\gamma_\alpha$. Hence $S_\alpha^2 = -I_n$, so each S_α determines a complex structure. Next we consider the $(p-2)$-dimensional sphere S^{p-2}. For a point $\tilde{n} \in S^{p-2}$, $\tilde{n} = (n_1, ..., n_{p-1})$ with $n_1^2 + ... + n_{p-1}^2 = 1$, we set

$$J_{\tilde{n}} = n_1 S_1 + ... + n_{p-1} S_{p-1}$$

which is also a complex structure. The complex structure $J_{\tilde{n}}$ is called the *supercomplex structure for the direction n.*

Finally, consider a separable Hilbert space H over the field of real numbers R. A pair (H, S) is called a pre-Hurwitz pair [30] if there exists a bilinear mapping $f: \mathrm{H} \times S \to \mathrm{H}$ satisfying

$$\|f(x, y)\|_{\mathrm{H}} = \|x\|_S \|y\|_{\mathrm{H}} \quad \text{for any } x \in S \text{ and } y \in \mathrm{H},$$

where $\| \ \|_S$ and $\| \ \|_{\mathrm{H}}$ denote the norms of S and H, respectively. A pre-Hurwitz pair is called *decomposable*, if H has the decomposition

$$\mathrm{H} = \oplus_{k=1}^{\infty} V_k, \quad \text{where } (V_k, S) \text{ are (euclidean) Hurwitz pairs.}$$

In this case, choosing complex structures J_k on V_k, we define a (*decomposable*) *supercomplex structure* J on H by

$$J = \oplus_{k=1}^{\infty} J_k.$$

6. UNIFICATION OF VARIOUS TYPES OF HYPERFINE INTERACTIONS

The concept of unification of various types of hyperfine interactions, originated in [5, 6] and further developed in the present paper, involves the use of Finsler geometry and supercomplex structures.

In Section 3 we have already noticed that in certain cases the equation of motion has solutions. On the other hand, as remarked in Section 4, it is clear that, in contrast to Riemannian geometry, in the Finsler geometry all the solitons are solutions of the equations of motion, i.e. of the Euler-Lagrange equations. Consequently, these equations can be regarded as

$$(\partial/\partial\delta)[u_t(\partial/\partial u_\delta)F=0, \quad \text{where } u=u(\delta,t), \quad F=F(u,u_t,u_\delta), \tag{7}$$

and then compared, for instance, in the case of ferroelectric crystals, with the results of [26, 27].

Besides, in order to derive the hamiltonians involved in the intrinsic symmetries, we shall apply the concept of supercomplex structure given in Section 5. Our motivation is the following: The success of the complex analysis has already been caused by the decomposition

$$(x_1^2+x_2^2)(y_1^2+y_2^2)=(x_1y_1-x_2y_2)^2+(x_1y_2+x_2y_1)^2, \tag{8}$$

where x_1 etc. are real. Unfortunately, an analogous problem of $x_1^2+x_2^2$ being replaced by $x_1^2+x_2^2+x_3^2-x_0^2$ has no solution, but is solvable if we go over to the *Kałuża-Klein theories*: $\|x\|^2=x_1^2+\ldots+x_{8k+4}^2-x_0^2$, where $k+1$ is a positive integer [31], interpreted as the number of particles [6].

Therefore, considering the inclusion of the hyperfine interactions to the hamiltonian, we follow the spirit of the Kałuża-Klein theory of arbitrary order $p=8k+5$. We shall now investigate a generalised Breit equation, including the pseudo-riemannian geometry (which can easily be replaced by a Finsler geometry, as indicated in Section 4) and the Clifford structures in the form of Hurwitz pairs and the related supercomplex structures. This approach leads to further types of interactions connected with the richness of the Clifford algebras and reflecting the intrinsic symmetries of the system.

For instance, already in the case of two particles ($k=1$), in contrast to the usual Pauli theory [32], instead of two systems of spin we have $2^{4k}=16$ systems of reduced spins. Two of them correspond to the two particles in question, in our case to two electrons, while the others to 14 types of interactions. Explicit formulae will be given in the next section, showing that the additional spins enable us, in contrast to the Pauli theory, to preserve linearity in the sense of the Dirac programme concerning the one-particle problem.

7. GENERALISED BREIT EQUATIONS – HEURISTIC INTRODUCTION

Consider a particle in space, treated as the *space of the particle*. In the simplest case it is euclidean space with the orthonormal basis (e_j), $e_je_k=\delta_{jk}$ (the Kronecker symbol). If the particle has mass and charge, we deal with gravitational, electromagnetic, strong and weak fields in the particle space. The particle couples with these fields, described by Dirac-Maxwell and Yang-Mills equations. Its equation of motion, of the form

$$m\ddot{\underline{x}} = \mathcal{F}(t, \underline{x}, \dot{\underline{x}}),$$

includes the influence of those fields on the motion of the particle. We see that even in so simple a case as that of an individual elementary particle, the suitable equations are quite complicated.

Assume for a moment that the particle has only mass. The case has been considered by Einstein who discovered that one can obtain a correct equation for the particle space without gravitational field, albeit with a non-euclidean metric. This can be understood as the space of *observations* of the particle. The curvature of the space is connected with mass. By analogy to general relativity, we can construct the particle space whose geometry describes all four fields.

Consider, in particular, a vector space with basis (ε_j). The familiar formula $g_{jk}=(e_j, \varepsilon_k)$ gives the matrix of coefficients, called the metric of the space.

In our general case, the metric is supposed to be complex:

$$g = g_e + ig_n.$$

The first part expresses the electromagnetic field and the other the nuclear one. There are many metrics with those properties. We choose that which gives the Dirac-Maxwell and Yang-Mills fields in the form of equations compatible with Dirac-Maxwell system. Under those assumptions the particle is described by the system

$$D\underline{\Psi}=0, \quad \Box\underline{\Gamma}=-ie\underline{j}, \quad \operatorname{Div}\underline{\Gamma}=0; \quad \underline{\Gamma}=\underline{\Gamma}^n-i\underline{\Gamma}^e, \tag{9}$$

where D is the Dirac operator corresponding to the electromagnetic and nuclear fields, and j is the current generated by $\underline{\Psi}$. $\underline{\Gamma}^n$ and $\underline{\Gamma}^e$ are the spinor connections and $e=e_0/\hbar c$, where e_0 denotes the electric charge of the electron.

Then, in [6], a complex-analytical method of solving the system (9), based on linearization of the spinor connections, is given, which is equivalent to linearization of the metric of the space.

In a more general case, the external fields are not only self-electromagnetic and self-nuclear but, moreover, have to be considered the ones coming from the other particles in the same space, like in a crystal or in a solid state sample.

Thus, we have to turn our attention to the construction of an equation for a system of mutually interacting particles. Let us concentrate on an arbitrary many-electron system in an external field. Irrespective of whether we are dealing with a thin film or a bulk, with an interior atom or an adatom with their nearest neighbours, we are interested in a system of $k+1$ electrons. If these electrons belong to n atoms, we have a decomposition $k+1=k_1+\ldots+k_n$.

In 1930 G. Breit gave his equation for a two-particle system

$$\left(E-H_{(1)}-H_{(2)}-\frac{e_0^2}{r_{12}}\right)U=-\frac{e_0}{2r_{12}}\left[\underline{\alpha}_1\cdot\underline{\alpha}_2+\frac{(\underline{\alpha}_1\underline{r}_{12})(\underline{\alpha}_2\underline{r}_{12})}{r_{12}^2}\right]U, \tag{10}$$

where E is the total energy: $EU = \hbar c \partial^0 U$, $H_{(1)}$ and $H_{(2)}$ are the Dirac hamiltonians corresponding to each of the two particles alone, $\underline{\alpha}_1$ and $\underline{\alpha}_2$ are the corresponding Dirac matrices, $\underline{r}_1$ and $\underline{r}_2$ are the positions of two electrons on which the wave function U depends, and r_{12} is the distance between the two electrons, while $\underline{r}_{12} = \underline{r}_1 - \underline{r}_2$.

A relativistic approach to the many-electron problem as a generalisation of the Breit equation for a many-particle case leads to the Dirac-Maxwell system. It has the form resembling the one-particle case:

$$\tilde{D}^q \underline{\Psi}^q = 0; \quad \Box_p \Gamma^q = -ie\underline{j}^q; \quad \mathrm{Div}_p \Gamma^q = 0, \quad \text{where } p = 8k+5, \tag{11}$$

and

$$\tilde{D}^q = D^q + (2/\hbar c)\hat{H}^q_{\mathrm{int}}, \quad q \leqslant k+1,$$

where D^q is the Dirac operator corresponding to the q-th particle alone, $\underline{j}^q$ is the current generated by $\underline{\Psi}^q$, $(2/\hbar c)\hat{H}^q_{\mathrm{int}}$ denotes the interaction part of D^q, and Γ^q is the corresponding spinor connection [6].

8. GENERALISED BREIT EQUATIONS AND DIRAC-MAXWELL SYSTEMS IN SUPERCOMPLEX GEOMETRY

We are going to formulate the previous considerations concerning the generalised Breit equations and the related hamiltonians in a more precise way.

According to the results of [6], by [33, 34, 5], the relativistic approach to the many-particle problem as a generalisation of the Breit equation (10) leads to a system of Dirac-Maxwell-like equations (11), where

$$\tilde{D}^q = D^q + (2/\hbar c)(\gamma^{q0} + I_\nu)^{-1} H^q_{\mathrm{int}}, \quad q \leqslant k+1, \tag{12}$$

$D^q = \gamma^{q0} H^q$, H^q is the hamiltonian and γ^{qj}, $j = 0, \ldots, p-1$, are generators of the Clifford algebra corresponding to the q-th electron, $q = 1, \ldots, k+1$; and

$$H^q_{\mathrm{int}} = (\hbar e c)^2 \sum_{j \neq q} \frac{1}{r_{jq}} (I_\nu - \tfrac{1}{2} \underline{\alpha}^j \underline{\alpha}^q) + H_{\mathrm{dem}},$$

$$H^q_{\mathrm{dem}} = \tfrac{1}{2}(\hbar e c)^2 \sum_{j \neq q} \frac{1}{r^3_{jq}} (\underline{\alpha}^j \underline{r}_{jq})(\underline{\alpha}^q \underline{r}_{jq}).$$

Here, I_ν stands (as before) for the identity $\nu \times \nu$-matrix, $\nu = 2^{4k+3}$, $\underline{r}^q = ie\underline{A}^q$ is the spinor connection, $\underline{A}^q$ denotes the self-electromagnetic field of the q-th electron, $\underline{r}_{jq}$ stands for the euclidean vector between the j-th and q-th electrons, and r_{jq} for their euclidean distance. Similarly, $\underline{\alpha}^q$ denotes the coefficient matrix for (γ^{jq}):

$$\gamma^{jq} = \alpha^{jq}_i \gamma^{iq}_0.$$

From (12) we see that the total hamiltonian H is the sum of the hamiltonians H^q and H^q_{int}:

$$H=\sum_q (H^q+H^q_{\text{int}}),$$

where H^q is the hamiltonian of the q-th individual electron and H^q_{int} is the part of the hamiltonian corresponding to the interactions between the q-th electron and the remaining ones; it includes the demagnetizing term H^q_{dem}.

Now, we consider the Hurwitz pairs $(S, V)=(\{x\}, \{y\})$, discussed in Section 6 in connection with generalisations of (8) in the spirit of the generalised Hurwitz condition (6), and generalise the concept replacing S by a suitable fibre bundle $\mathscr{B}_{\mathrm{M}}$, where M denotes the fibre space. The mathematical details of the procedure are given in [6]. (In the case of one particle, $k=0$, M can be chosen as the Cartesian product of the Minkowski space-time and the circle whose curvature is interpreted as the mass.) Then we consider the eigenvalue problem concerning the equation

$$Jf=z\cdot f \quad \text{for} \quad f\in V, \tag{13}$$

where $T_z\mathrm{M}\times V\to V$ is the multiplication, $T_z\mathrm{M}$ denotes the complexified space tangent to M at z, and J is the endomorphism corresponding to a complex structure of $T_z\mathrm{M}$; cf. Section 5. The system corresponding to the intrinsic symmetries of the pseudo-riemannian Hurwitz pair $(\mathscr{B}_{\mathrm{M}}, V)$, $\dim \mathrm{M}=p$, $\dim V=\nu$, is connected with the hamiltonian including interactions of higher orders with respect to the operators of annihilation and creation of electrons.

Consider the system (9) with the operators (10), which now reflects the intrinsic symmetries of the *supercomplex geometry* of $(\mathscr{B}_{\mathrm{M}}, V)$. The corresponding hamiltonian includes interactions of higher orders with respect to the operators of annihilation and creation of electrons. We reduce the system of $k+1$ interacting electrons coming from the n atoms in question to the system of $k+1$ free electrons considered individually in the external 2^{4k+3}-dimensional field caused by the remaining electrons, as described by the general Dirac-Maxwell system. Next, we multiply both sides of the Dirac-type equations in the system (11) by suitable conjugate operators

$$\bar{D}^q=\bar{D}^q_0+\bar{D}^q_1-ie^{q0}_\gamma A^{q0}, \quad \text{where } \bar{D}^q_0=-D^q_0 \quad \text{and } \bar{D}^q_1=-D^q_1+2I_\nu m,$$

where $m=m_0 c/\hbar$ and m_0 denotes the rest mass of the electron. For the nonrelativistic *energy* $W=\sum W^q$ *of the system* we get a relativistic expression of the form

$$W=B_2(H_{\text{int}})+B_4(H_{\text{int}})+B_6(H_{\text{int}})+o(|H_{\text{int}}|^3), \quad H_{\text{int}}=\sum H^q_{\text{int}}, \tag{14}$$

where B_2, B_4 and B_6 are the terms of the second, fourth and sixth orders with respect to $(H_{\text{int}})^{1/2}$ or, equivalently, with respect to the operators of creation and annihilation of electrons [6].

The expressions obtained for the energy $W=\sum W^q$ of the system of electrons, placed in a field characterized by the geometry corresponding to the pseudo-riemannian Hurwitz pair $(\mathscr{B}_{\mathrm{M}}, V)$ in question, provide us with a starting

point for describing the system in terms of second quantization. Following the usual procedure of the second quantization we arrive at an expression for the hamiltonian H, associated with the energy W, in the form

$$H=\sum_{\lambda,\lambda'} t_{\lambda\lambda'}\, a_\lambda^+ a_{\lambda'} + \tfrac{1}{2}\sum_{\lambda\rho\rho'\lambda'} I_{\lambda\rho\rho'\lambda'}\, a_\lambda^+ a_\rho^+ a_{\rho'} a_{\lambda'} + \tfrac{1}{4}\sum_{\lambda\rho\varkappa\varkappa'\rho'\lambda'} L_{\lambda\rho\varkappa\varkappa'\rho'\lambda'}\, a_\lambda^+ a_\rho^+ a_\varkappa^+ a_{\varkappa'} a_{\rho'} a_{\lambda'} + o(\|a_\lambda^+ a_{\lambda'}\|^3), \tag{15}$$

where a_λ^+ resp. a_λ denote the creation and annihilation operators, while the matrix elements $t_{\lambda\lambda'}$, $I_{\lambda\rho\rho'\lambda'}$ and $L_{\lambda\rho\varkappa\varkappa'\rho'\lambda'}$ contain the one-, two- and three-particle interactions, chosen according to the formula (14).

An analysis of the expressions (14) and (15) shows that the linear dependence of the energy of the *hyperfine interactions* on the values of electron and nuclear spins holds with accuracy to $(|H_{\text{int}}|^{3/2})$ or, equivalently, to $o(\|a_\lambda^+ a_{\lambda'}\|^{3/2})$. Therefore in strong fields there may occur nonlinear interactions, foreseen in a natural way by the theory.

9. LANGEVIN-TYPE EQUATIONS IN SUPERCOMPLEX GEOMETRY

As it has been observed in [20], the Langevin-type equations including the electron, phonon, and electron-phonon vibrations can be derived from the intrinsic symmetries of $(\mathscr{B}_M, V)$; however, an effective construction is only initiated in [6].

Precisely, in the case of a chain of atoms in a crystal, we have

$$H=H_e+H_p+H_{ep}, \tag{16}$$

where H_e is caused by the electronic vibrations, H_p by phonon vibrations, and H_{ep} by the electron-phonon coupling:

$$H_e=\sum_{\lambda,\bar\lambda} t_{\lambda\bar\lambda}\, a_\lambda^+ a_{\bar\lambda} + \tfrac{1}{2}U\sum a_{\lambda(\sigma)}^+ a_{\lambda(\sigma)} a_{\lambda(-\sigma)}^+ a_{\lambda(-\sigma)} - \mu\sum a_\lambda^+ a_\lambda,$$

$$\lambda=(\nu,j,m,\sigma) \quad \text{and} \quad \lambda+1=(\nu,j+1,m,\sigma),$$

$$H_p=\tfrac{1}{2}M\sum_j p_j^2+\tfrac{1}{2}a\sum_j (R_{j+1}^2-R_j^2)+\dots,$$

$$H_{ep}=I\sum_j (R_j-R_{j+1})(a_\lambda^+ a_{\lambda+1}).$$

The expressions are written in standard notation in the Hubbard approximation applied to (15) together with the pseudoharmonic approximation [17].

From the viewpoint of the *deformation of the metric*, in particular in near-surface regions, the procedure leads to a positive solution of the problem, posed in [17], whether a generalised Langevin equation (1) or its counterpart, resulting from the hamiltonian (16), can be transformed to a Langevin equation by including the stochastic force $\mathscr{F}(t)$ ȯf (1) in a suitably curved geometry.

Of course, the simplest case occurs when we confine ourselves to the phonon vibrations. This is the case when the vibrational properties of ultra-heavily doped *semiconductors* are discussed [34]. In the next section, continuing the ideas of the microscopic electronic theory of paramagnetic Co_xFe_{1-x} alloys [7], we shall give an application of our approach to paramagnetic binary alloys of the type A_xB_{1-x}, including more general interactions: of the second and third orders.

One step further is a consideration of the hyperfine interaction in connection with the *electronic band structure* of thin films of semiconductors like CdTe [36], in particular the *dependence* of that structure on *temperature*, and with the *photoreflectance* of radiofrequency sputtered thin films, for instance $Cd_{1-x}Fe_xTe$, $x=0.00$, 0.05, 0.10 and 0.15 [37]. As far as paramagnets of the rare earths are concerned, in the Instituto Politecnico Nacional, Mexico, ceramic oxides are being studied [25]. Here L is a rare earth, M = Sr or Ba, N = Cn and $6 \leqslant y \leqslant 6.5$. These materials become *diamagnets* at low temperatures according to the superconducting character of these ceramics, as well as the Perovskite structures mentioned in Section 3.

In Poland, rich material in this direction may be found in several papers written or inspired by Profs. W. Pajewski and Z. Surowiak [38, 39], in particular in connection with ferroelectrics.

10. APPLICATION TO PARAMAGNETIC BINARY ALLOYS OF THE TYPE A_xB_{1-x}

According to [7], the microscopic theory of paramagnetic Co_xFe_{1-x} alloys is based on adapting the tight-binding hamiltonian in the Bethe lattice approximation

$$H=\sum_{\alpha} \varepsilon_{\alpha} a_{\alpha}^{+} a_{\alpha}+\sum_{\beta} \varepsilon_{\beta} a_{\beta}^{+} a_{\beta}+\sum_{\alpha \neq \beta} t_{\alpha\beta} a_{\alpha}^{+} a_{\beta}+o(|H_{\mathrm{int}}|), \tag{17}$$

where the alloy is supposed to have N lattice sites subdivided into two equivalent sublattices α, β so that there are $\frac{1}{2}N$ sites of type α and $\frac{1}{2}N$ sites of type β labelled by α and β, respectively. Each α-site has Z sites of type β as its nearest neighbours and *vice versa*. We set

$$\sum_{\alpha}=\sum_{\alpha=1}^{\frac{1}{2}N}, \quad \sum_{\beta}=\sum_{\alpha=\frac{1}{2}N+1}^{N}, \quad \sum_{\alpha \neq \beta}=\sum_{\alpha=1}^{N} \sum_{\beta=1}^{N}.$$

Following the approach in Sections 6 and 7, by the formulae (14)–(16), the hamiltonian (17) has to be improved by the term

$$\begin{aligned}\Delta H=&\sum_{\alpha} \Gamma_{\alpha}(a_{\alpha}^{+} a_{\alpha})^2+\sum_{\beta} \Gamma_{\beta}(a_{\beta}^{+} a_{\beta})^2+\sum_{\alpha \neq \beta} I_{\alpha\alpha\beta\beta} a_{\alpha}^{+} a_{\alpha} a_{\beta}^{+} a_{\beta}\\ &+\sum_{\alpha} \Delta_{\alpha}(a_{\alpha}^{+} a_{\alpha})^3+\sum_{\beta} \Delta_{\beta}(a_{\beta}^{+} a_{\beta})^3\\ &+\sum_{\alpha \neq \beta} L_{\alpha\alpha\alpha\beta\beta}(a_{\alpha}^{+} a_{\alpha})^2(a_{\beta}^{+} a_{\beta})+\sum_{\alpha \neq \beta} L_{\beta\beta\beta\beta\alpha\alpha}(a_{\beta}^{+} a_{\beta})^2(a_{\alpha}^{+} a_{\alpha})\\ &+o(|H_{\mathrm{int}}|^3).\end{aligned} \tag{18}$$

The electronic energy levels of atoms situated in the α and β sublattices, denoted by $[\alpha]$ and $[\beta]$, take values ε_A resp. ε_B with the probabilities p_A^ν resp. p_B^ν, where $\nu=[\alpha]$ in the case of ε_α, and $\nu=[\beta]$ in the case of ε_β. The values Γ_A and Δ_A resp. Γ_B and Δ_B are taken with the probabilities p_A^ν resp. p_B^ν with analogous restrictions.

The interaction energy increments $t_{\alpha\beta}$ of those atoms take values t_{AA}, t_{BB} and $t_{AB}=(t_{AA}\,t_{BB}{}^B)^{1/2}$ with the probabilities $p_{AA}^{[\alpha\beta]}$, $p_{BB}^{[\alpha\beta]}$, and $p_{AB}^{[\alpha\beta]}$, respectively, where $[\alpha\beta]$ stands for $[\alpha]\,[\beta]$ etc. The interaction energy increments $I_{\alpha\alpha\beta\beta}$ of those atoms take values I_{AAAA}, I_{BBBB}, $I_{AABB}=(I_{AAAA}\,I_{BBBB})^{1/2}$ and $I_{AAAB}=(I_{AAAA}^3\,I_{BBBB})^{1/4}$ with the probabilities $p_{AAAA}^{[\alpha\alpha\beta\beta]}$, $p_{BBBB}^{[\alpha\alpha\beta\beta]}$, $p_{AABB}^{[\alpha\alpha\beta\beta]}$ and $p_{AAAB}^{[\alpha\alpha\beta\beta]}$, respectively. Analogous formulae for the interaction energy increments of higher order will be published in [8].

The probabilities in question are subjected to the constraints

$$\sum_{I,J} p_{IJ}^{[\alpha\beta]}=1 \quad \text{for } I,J=(A,A),\ (B,B),\ (A,B),\ (B,A),$$

$$\tfrac{1}{2}(2p_{AA}^{[\alpha\beta]}+p_{AB}^{[\alpha\beta]}+p_{BA}^{[\alpha\beta]})=x,$$

$$\tfrac{1}{2}(2p_{AAAA}+p_{AAAB}+p_{AABA}+p_{ABAA}+p_{BAAA}+p_{ABBB}$$
$$+p_{BABB}+p_{BBAB}+p_{BBBA}+p_{ABAB}$$
$$+p_{ABBA}+p_{BBAA}+p_{BABA}+p_{BAAB})=x,$$

where in the last formula we have set $p_{AAAA}=p_{AAAA}^{[\alpha\alpha\beta\beta]}$, etc. An analogous formula for the higher order probabilities will be published in [8]. The above formulae and the explicit form of (14), given in [6] (formulae (44)–(45)), show that from the viewpoint of magnetic interactions the contribution of the third addend (containing the energy increments $I_{\alpha\alpha\beta\beta}$) on the right-hand side of (18) gives a contribution to ΔH lower by one order than the contribution of the remaining addends.

The local Green functions $G^{I\nu}(\omega)$, calculated from the equations of motion [7]:

$$(\omega-\varepsilon_A)\,G_{00}^{A\nu}=1+Z\left(\frac{p_{AA}^{\nu\mu}}{p_A^\nu}\,t_{AA}\,G_{10}^{A}+\frac{p_{AB}^{\nu\mu}}{p_A^\nu}\,t_{AB}\,G_{10}^{B\mu}\right),$$

$$(\omega-\varepsilon_A)\,G_{00}^{A\mu}=\ldots,\quad (\omega-\varepsilon_B)\,G_{00}^{B\mu}=\ldots,\quad (\omega-\varepsilon_B)\,G_{00}^{B\mu}=\ldots,$$

where $\mu=[\alpha],[\beta]$ and $\nu=[\alpha],[\beta]$, give the local density of states

$$N_{I,\nu}(\omega)=-(1/\pi)\,\mathrm{Im}\,G_{00}^{I\nu}(\omega),\quad I=A,B, \tag{19}$$

the total average density of states

$$N(\omega)=\tfrac{1}{2}N\sum_{I,\nu}\rho_I^\nu N_{I,\nu}(\omega), \tag{20}$$

and the configurational entropy which, in the Bethe approximation, is expressed as

$$S=kN\left\{\tfrac{1}{2}(Z-1)\sum_{I,\nu}p_I^\nu\ln p_I^\nu-\tfrac{1}{2}Z\sum_{I,J}p_{IJ}^{[\alpha\beta]}\ln p_{IJ}^{[\alpha\beta]}\right\}.$$

Analogous equations and formulae including increments of higher order will be published in [8].

11. THE SECOND QUANTIZATION AND OGUCHI'S THEOREM IN SUPERCOMPLEX GEOMETRY

With the energy (14) we have associated, as usual, the hamiltonian (17) determined with respect to the operators of creation and annihilation of electrons *via* expanding the wave function into a series of eigenfunctions constituting a system of solutions of the system (11). The study of the term B_6 in the formula (14) gives a theoretical proof of the *dependence of the band structure on temperature* with a possibility of numerical calculations.

Moreover, the formula (15) enables us, with an accuracy that can effectively be estimated, to verify the theorem, following from the Oguchi theorem concerning the equation (2), on the linear *dependence of the energy of the hyperfine interaction on* the values of electron and nuclear *spins* [23].

In the formulae (14) and (15) there also appear corrections to the *electron correlation functions*, describing the electron states density (cf. the way of obtaining the formulae (19) and (20)), which yield the charge density distribution, the work function, and the others characterizing the system of electrons.

The same calculation applies to the particularly interesting case of *autocorrelation of electrons* quite analogous to the autocorrelation in Section 1, which now describes the behaviour of an electron at two different instants, expresses delocalization of that electron and determines the finite time of its definite quantum state. Thus the related *autocorrelation time* describes the blurring of the process of delocalization of the electron and the reversal of spin orientation. As far as the nonrelativistic theory is concerned, the *spin autocorrelation*, corresponding to the two-particle autocorrelation of the type described by the product of $\exp[i(H/\hbar)t]$, $a^+_{r\uparrow}a_{r\uparrow} - a^+_{r\downarrow}a_{r\downarrow}$ and $\exp[-i(H/\hbar)t]$, $a^+_{r\downarrow}a_{r\uparrow} - a^+_{r\uparrow}a_{r\downarrow}$, is determined by a diffusion process.

Obviously, a further progress is connected with the inclusion of a relativistic approach in the hamiltonian (15). If in the formula (14), related to (15), we include the dependence on B_6 and the successive addends, and establish the influence of the higher order correlations on the *relaxation processes*. This proves the *spectrum line widening*, implemented also by autocorrelation time. The influence is of a more complicated character since it depends intrinsically on the temperature by the occurrence of the many-particle interactions.

The most natural way to investigate the temperature dependence of the many-particle interactions is to study the temperature dependence of the order parameters. Let us take again in the new context of ferromagnets the binary model with N lattice sites subdivided into two equivalent sublattices α, β such that there are $\frac{1}{2}N$ sites of type α and $\frac{1}{2}N$ sites of type β. With the same notation, it

is convenient, in the first order approximation, to consider a long-range order parameter

$$\eta := (p_{AA}^{[\alpha\beta]} + p_{AB}^{[\alpha\beta]}) - (p_{AA}^{[\alpha\beta]} + p_{BA}^{[\alpha\beta]}) = p_A^{[\alpha]} - p_A^{[\beta]}, \tag{21}$$

and a short-range order parameters

$$\sigma := 1 - \tfrac{1}{2}(p_{AB}^{[\alpha\beta]} + p_{BA}^{[\alpha\beta]})/x(1-x), \tag{22}$$

with the meaning of x analogous to that in Section 9.

12. SOLITARY WAVES IN SUPERCOMPLEX GEOMETRY

By [33, 34] we can see that the system (11) always generates a Kadomtsev-Petviashvili system having, in general, soliton solutions. Namely, with the operators (12) we associate the pseudo-differential operators

$$W_q(t) := I_v + u_q^1(z,t)(\tilde{D}^q)^{-1} + u_q^2(z,t)(\tilde{D}^q)^{-2} + \ldots, \quad z \in M,$$

where M is the fibre space constructed in Section 8 and $t = (t_1, t_2, \ldots)$ is a system of infinitely many parameters. Consider the *generalised lagrangians* $L_q(t) := W_q \tilde{D}_q W_q^{-1}$ (not being summed). Then each $L_q(t)$ determines an *isospectral deformation of* $\tilde{D}^q$: any eigenfunction λ_q of the equation

$$L_q(t)\Psi = \lambda_q \Psi \tag{23}$$

remains fixed, independently of the choice of t. The corresponding *Kadomtsev-Petviashvili* system reads:

$$\frac{\partial}{\partial t_n} L_q = [(L_q^n)_+, L_q], \quad n = 1, 2, \ldots, \quad \text{where } (L_q^n)_+ = \left(\frac{\partial}{\partial t_n} W_q\right) W_q^{-1} + L_q^n \tag{24}$$

and L^n is defined as $L^{n-1}L$.

The eigenvalue problem concerning (23) is closely related to the eigenvalue problem concerning (13). The relationship has recently been established partially in our joint paper [30]. Precisely, the positive answer is proved to hold for the decomposable supercomplex structures introduced in Section 6.

Before formulating the result, which seems to be quite important when studying solitary waves, especially *surface solitons*, we have to recall some basic facts on the reduction solutions of Kadomtsev-Petviashvili systems [40].

A solution of the Kadomtsev-Petviashvili system (24) is called an l-reduction solution if $(L^l)_+ = L^l$ for some integer l. For instance, 2-reduction solutions give rise to those of

$$u_t - 6uu_x + u_{xxx} = 0 \quad \text{(the Korteweg-de Vries equation)},$$

and 5-reduction solutions to those of

$$3u_{yy} + (u_{xxx} + 12uu_x)_x = 0 \quad \text{(the Boussinesq equation)}.$$

It is well known that l-reduction solutions can be characterized in terms of the

so-called *Kac-Moody Lie algebra*, more exactly the Lie algebra $A_{l-1}^{(1)}$ [41]. An element $\xi \in A_{l-1}^{(1)}$ can be expressed as

$$\xi = \sum_{k=-\infty}^{+\infty} X^{(k)} \lambda^k, \quad X^{(k)} \in sl(l, \mathrm{R}), \tag{25}$$

where λ is a parameter. In a similar manner we can define $\mathcal{G}$-reduction solutions. We choose a Lie subalgebra $\mathcal{G}$ of $sl(l, \mathrm{R})$ and ξ by (25) with $X^{(k)} \in \mathcal{G}$, $k \in \mathrm{Z}$. The corresponding solutions of the Kadomtsev-Petviashvili system (24) are called *$\mathcal{G}$-reduction solutions.*

Now, the relationship between the eigenvalue problems concerning the equations (13) and (23) can be formulated as follows: There exists a correspondence between a set of decomposable supercomplex structures and a set of $so(p-1)$-reduction solutions of the Kadomtsev-Petviashvili system (24). The above theorem still holds true in the case of pseudo-euclidean Hurwitz pairs (V, S), where the metric of V, analogous to the metric $(\ )$ of S, is finite-dimensional and, after diagonalization, has an even number of signs $+$ (or, equivalently, of signs $-$).

13. APPLICATION TO THE VIBRATIONAL PROPERTIES OF FERROELECTRICS

Consider an anharmonic crystal under the assumptions of Section 9. This means that the hamiltonian (15), derived from the intrinsic symmetries of the crystal, is given by (16) and includes electronic and phonon vibrations as well as the electron-phonon coupling.

The equations of motion, derived in [20] from (16) with the use of the Lindner-Fedyanin method, are of the form

$$M\ddot{x} = -\alpha x'' + \frac{2I}{a} \sum_{\sigma} \frac{\partial}{\partial \xi} (\Phi_{\sigma} \Phi_{-\sigma}), \quad \text{where } x = x(\xi, t), \tag{26}$$

and

$$j\dot{\varphi}_{\sigma} = T\Phi''_{-\sigma} + 2T\Phi_{-\sigma} - \frac{(2I)^2}{M(\omega^2 - \omega_0^2)} \sum_{\sigma'} \Phi^*_{\sigma'} \Phi_{-\sigma'} \Phi_{-\sigma}$$

$$+ U|\Phi_{-\sigma}|^2 \Phi_{\sigma} - 1T\Phi_{\sigma}, \quad \text{where } \omega_0 = \frac{\alpha}{M}. \tag{27}$$

The equations (26) and (27), in particular the third and fourth addends on the right-hand side of (27), give a starting point for discussing the *solitary waves* in the context of the theory of *layers near the surface* in anharmonic crystals. According to the sign of the coefficient U and $(2I)^2/M(\omega - \omega_0)^2$, the influence of vibrations determines the appearance of an electronic soliton. In consequence, according to the equation (26), the solution for vibrations $x(\xi, t)$ depends on the shape of the solution for φ_{σ} and $\varphi_{-\sigma}$.

As explained in Section 6, in order to place the phenomenon of solitons within some mechanics we have to go over from classical to Finsler mechanics and to consider the Euler-Lagrange equations (7). In the case of single solitons and one-wall motion in elastic ferroelectrics in the presence of electromechanical couplings, the equations of motion become

$$Qu_{tt}=\hat{c}_{\|}\,u_{xx},$$
$$Qv_{tt}-c_{\perp}\,v_{xx}=-e\theta_x\cos 2\theta,$$
$$J\theta_{tt}-K\theta_{xx}=ev_x\cos 2\theta+\lambda\sin 2\theta;$$

cf. [26, 27], where the physical meaning of the parameter functions is given.

In the case of Bloch walls in an infinite crystal, the solitary waves are solutions of a simple sine-Gordon equation $u_{xt}=\sin u$. In the case of Néel walls in a thin elastic wall, the magnetic-spin orientation remains nonlinearly coupled with the elastic displacement polarized in the plane of the film. Therefore we have to deal with a nonlinearly coupled system of sine-Gordon or a double sine-Gordon equation (3), where γ is a real constant. For $\gamma=0$, (3) reduces to the sine-Gordon equation and the one-soliton solutions of (3) read

$$u_1=-2\arctan\left[a\sin h(x-\omega t)\right],\qquad u_2=\pi-2\arctan\left[a\sin h(x-\omega t)\right],$$

where ω is a constant and $a=(1+2\gamma)^{-1}$. As a more sophisticated example of (7), in [20] the soliton equation

$$u_t\,u_x=2u_{tx}\tan\tfrac{1}{2}u$$

is considered on the surface.

An interesting case of the theory takes place for ferroelectric crystals of the KDP, TGS, and related types. In the case of KDP, given as $KDPO_4$, we take into account [11] in analogy with a crystalline binary alloy of type $G_{1-x}P_x$ containing electrically inactive ions P_1 (trigonal sites) and electrically active ions P_2 (tetragonal sites) [9]. In our case we set $P_1=D_{\downarrow}^{+}$ and $P_2=D_{\uparrow}^{+}$, so that P_1 and P_2 correspond to two sides of the planes determined by O_4 in the associated ions PO_4^{-}. The role of atoms G is to be fulfilled here by the sites with complete order, but with some average displacement η in the sense of [10], formulae (2.12). In the case of TGS, given as $(NH_2CH_2COOH)_3H_2SO_4$, the situation is quite similar. We take $P_1=H_{\downarrow}^{+}$ and $P_2=H_{\uparrow}^{+}$, so that P_1 and P_2 correspond to two sides of the planes determined by O_4 in the associated ions SO_4^{-}. The definition of G remains unchanged.

In the general case of a ferroelectric crystal, as considered in [10], it is assumed that there are two basic kinds of phase transitions, the one being of the *order-disorder type*: (P_1, P_2), and the other of the *displacive type* G. In the first case the phase transition is a consequence of statistical disorder of active atoms among several equilibrium positions determined for each cell by the remaining atoms; we restrict ourselves to the simplest case of two types of positions P_1 and

P_2. In the latter case (concerning G) the phase transition is caused by lattice instability against a certain atomic vibrational mode.

In analogy to the previous cases in question, the model quoted can be derived from the intrinsic symmetries of the system by the general approach proposed in [6], where the equations of motions, related to the crystallographic lattice, are understood in the statistical sense [17, 21]. Precisely, two order parameters, associated with the motion of active atoms, can be distinguished (cf. [10]): the temperature-dependent average population $\sigma_\alpha(T)$ for one of two equilibrium positions $\alpha = +, -$, corresponding to the pseudospin approach, and the average displacement $\eta_\alpha(T)$ with respect to the centre of the cell, corresponding to the self-consistent phonon scheme. Then, the order-disorder type of phase transition occurs when $\sigma_+(T)=\sigma_-(T)$ and the displacive type when $\eta_+(T)=\eta_-(T)=0$.

The parameter x appearing in the notation $G_{1-x}P_x$ for the alloy type considered in [9] is to be replaced here by the spontaneous polarization P_s of order-disorder type [10], formula (4.10), as follows [11]: In [9] we had $x=x_1+x_2$, $x_1=N'/N_P$ and $x_2=N_P/N$, where N'_P denoted the number of electrically inactive ions P_1, N_P the number of electrically active ions P_2, and N the total number of sites in the alloy. In the case of a ferroelectric with phase transitions of the order-disorder type (P_1, P_2) and the displacive type G we set $x_1-x_2=xP_s$, $x_1+x_2=x$. Hence it is natural to consider the ferroelectric analog of A_xB_{1-x} with

$$x_1=\tfrac{1}{2}x(1+P_s), \quad x_2=\tfrac{1}{2}x(1-P_s), \quad P_s\leqslant 1. \tag{28}$$

Now, a Born-type hamiltonian can be used [11] in order to calculate the density of states at a given site in real space. Special attention has to be paid to sites in near-surface regions, including the differences in distribution of the nearest neighbours. Taking into account all the possibilities concerning the pseudospin operator at trigonal and tetragonal sites, the hamiltonian deduced from the general formula (15) coincides with that proposed in [10]. Higher order terms can be included here in accordance with [6], where they are derived *via* expressing the hyperfine structure by the internal symmetries in terms of Dirac-like supercomplex structures. In particular, the density of states can be calculated within the theory of heavily doped semiconductors, applied to ferroelectrics based on the corrected Born-type hamiltonian, with the use of the Green function method. On the other hand, the same quantity can be derived from the Pouget-Maugin theory [26, 27], which gives another Green function yielding the electroacoustic density of states. Still, a Green function can be calculated independently by [10]. These procedures enable us to compare those three quantities and, more generally, the models, in addition to their comparison with experiment.

14. APPLICATION TO RAMAN SCATTERING IN NEAR-SURFACE REGIONS

The basic formula (15) for the total hamiltonian can be applied both in the case of Raman and Brillouin scattering. In analogy to the case of paramagnetic binary alloys considered in Section 10, by the explicit form of (14) given in [6], formulae (44)–(45), it can be shown that the two-step iteration for the energy W, described in Section 8, is quite satisfactory when deriving the semi-phenomenological formula for the Raman scattering efficiency due to Irmer *et al.* [42]. More careful calculations give even some improvement as far as the electron-phonon coupling is concerned; cf. the term H_{ep} in the formula (16). Since detailed calculations have not been completed yet, we shall publish them separately.

The present stage of development relates well to several theoretical results, both for the bulks and near-surface layers [43–47]. In the context of Raman scattering the efficiencies I_A and I_B are given by the formulae

$$I_A = \frac{d^2S}{d\omega\, d\Omega}\bigg|_A = \frac{16\pi\hbar n_2}{V_0^2 n_1}\,\frac{\omega_2^4}{C^4}\left(\frac{d\alpha}{dE}\right)^2 (n_\omega + 1)\,\mathrm{A}\,\mathrm{im}\left(-\frac{1}{\varepsilon}\right), \tag{29}$$

and

$$I_B = \frac{d^2S}{d\omega\, d\Omega}\bigg|_B = R^2\,\frac{\hbar n_2}{\pi n_1}\,\frac{\omega_2^4}{C^4}\left(\frac{eq\mu}{\omega_1\,\omega_2}\right)^2 (n_\omega + 1)\,\mathrm{B}\,\mathrm{im}\left(-\frac{1}{\varepsilon}\right), \tag{30}$$

where, in addition to the standard notation, we have

$$\mathrm{A} := 1 + 2C\,\frac{\omega_t^2}{\Delta}\left[\omega_t^2\gamma(\omega_t^2-\omega) - \omega^2\Gamma(\omega^2+\gamma^2-\omega_t^2)\right]$$

$$+ C^2\,\frac{\omega_t^2}{\Delta(\omega_p^2-\omega_t^2)}\left\{\omega_p^2\left[\gamma(\omega_p^2-\omega_t^2) + \Gamma(\omega_p^2-2\omega^2)\right] + \omega^2\Gamma(\omega^2+\gamma^2)\right\}$$

$$\Delta := \omega_p^2\gamma\left[(\omega_t^2-\omega^2)^2 + (\omega\Gamma)^2\right] + \omega^2\Gamma(\omega_t^2-\omega_1^2)(\omega^2+\Gamma^2),$$

$$\mathrm{R} := \frac{Eg}{Eg - (h\omega_1)^2},$$

$$\mathrm{B} := \frac{1}{\Delta}\,\omega_p^2\gamma(\omega_t^2-\omega_1^2)^2 + \omega_p^4\Gamma(\omega_t^2-\omega^2) + \gamma\Gamma^2\omega_p^2\omega.$$

The Faust-Henry coefficient C is determined in the equation

$$\frac{I_{LO}}{I_{TO}} = \left(\frac{\omega_1+\omega_t}{\omega_1-\omega_t}\right)^4 \frac{\omega_1}{\omega_4}\left(1 + \frac{\omega_t^2-\omega_2^1}{C\omega_t^2}\right)^2.$$

The dielectric function ε is given by a sum of the contributions from the phonon and plasmon:

$$\varepsilon = \varepsilon_\infty\left[1 + \frac{\omega_L^2-\omega_t^2}{\omega_t^2-\omega^2-i\omega\Gamma} - \frac{\omega_p^2}{\omega(\omega+i\gamma)}\right],$$

where ω_p is the plasmon frequency: $\omega_p^2 = 4\pi ne^2/\varepsilon_\infty m^* c$, while ω_t and ω_L are the frequencies of TO and LO phonons, respectively, γ is the plasmon damping constant, n denotes the free carrier concentration, $\omega_{1,2}$ are the incident and scattered phonon frequencies, V_0 is the volume of the unit cell, $n_{1,2}$ are the refractive indices at $\omega_{1,2}$, n_0 denotes the Bose factor, c is the velocity of light, E is the longitudinal macroscopic energy field, α denotes the polarizability, q is the momentum transfer of electrons, μ is the reciprocal effective mass, and E_g denotes the band gap energy.

The formulae (29) and (30), confirmed by the experiment [43], show, in particular, that the scattering intensity of the coupled modes depends on the magnitude of the momentum transfer of electrons.

CONCLUSIONS

Finally, we list some conclusions that seem to be quite promising as far as further research is concerned.

1. There are several analogies between surface properties of different physical problems described in the paper, in particular between (i) the demagnetizing fields related to solitary waves and their propagation over the surfaces of ferroelectrics, and (ii) the distribution of the diffusion coefficients over the surfaces and the concentration distributions in the near-surface regions of paramagnetic and semiconductor binary alloys (Sections 10 and 13).

2. The mutual influence of these properties (interactions, fields) is a typical surface effect which affects the diffusion coefficients and concentration distributions in question. This surface effect proves that, in analogy to the demagnetizing fields for ferroelectrics or, more precisely, to the fields existing in the region over the surface, there is a theoretical motivation for experimentally-known electric fields existing over the surface of ferroelectrics.

3. When studying the vibrational properties of ferroelectrics, following [10], we have distinguished two temperature dependent order parameters η and σ, connected with long- and short-distance dependence, respectively. By the formulae (21) and (22) we get the complete analogy to the cases of the temperature dependent order parameters for ferromagnets (Section 11) and paramagnets (Section 10).

4. In the light of Conclusions 1 and 2, the Oguchi theorem (Sections 2 and 11) may be regarded as a counterpart of the effects mentioned in the conclusions: it is still a statement on distribution of the diffusion coefficients. Moreover, the reformulation of the theorem in terms of supercomplex geometry points out additional analogies as far as the intrinsic symmetries of the system are concerned.

5. It is obvious that a deformation of a classical string with distinct ends, topologically equivalent to a closed line segment, to a classical string without ends, topologically equivalent to a circle, is a good model of small changes of the

system which, from the viewpoint of the bounding surface or of the boundary conditions on the boundary surface, leads to an entirely different behaviour of solutions of wave equations: non-periodic and periodic solutions, plane waves, solitons and instantons. As observed in [20], Section 4, the problem is intrinsically connected with the problem of irreducibility of the Hurwitz pair involved; cf. Section 5 of the present paper.

6. From the point of view of surface and near-surface regions we may say, regarding Conclusion 5, that the boundary conditions can be expressed in terms of deformation of the metric in near-surface regions. More precisely, in the case of a (pseudo-euclidean) Hurwitz pair (V, S) we have two related metrics and the induced supercomplex structure (J, z) corresponding at the same time to the generalised Breit equations (11)–(12). Any isospectral deformation of (J, z) is considered in relation to the eigenvalue problem concerning the equation (13).

7. From the viewpoint of the existence of surface solitary waves, the generalised Breit equations (11)–(12) induce a Kadomtsev-Petviashvili system (24) with respect to the generalised lagrangians $L_q(t)$. Any isospectral deformation of $L_q(t)$ is considered in relation to the eigenvalue problem for the equation (23).

8. In Section 10, the probabilities p_A^v, p_B^v, etc., depend on the position with respect to the surface of the paramagnetic binary alloy. This dependence is then reflected by the related supercomplex structure (J, z), the generalised lagrangians $L_q(t)$, the local Green functions $G^{Iv}(\omega)$, and the configurational entropy S. The problem is self-consistent: Since S has to attain its maximum, this property has to be implied by the proper distribution of atoms, i.e. by the proper concentration of the components A and B in the alloy A_xB_{1-x}. The role of an isospectral deformation is played here by an isoentropic deformation in which S always attains its maximal value. By Conclusions 1 and 2 the observation has its counterpart for ferroelectrics. We can take into account the spontaneous polarization P_S of order-disorder type and consider a ferroelectric of the type A_xB_{1-x}, $x=x_1+x_2$, with x_1 and x_2 given by (28).

9. Finally, let us return to the problem of including the three-body interactions (18) in the hamiltonian (17) for paramagnetic binary alloys A_xB_{1-x}. A further study of the formulae (44–(45) given in [6] can be done [11] in the case where, on the surface and in near-surface regions, the surface correlations give a contribution to (18) lower than the contribution of the internal correlations by one order. Then it appears that the contribution of the addends on the right-hand side of (18) containing the energy increments $L_{\alpha\alpha\alpha\beta\beta}$ and $L_{\beta\beta\beta\beta\alpha\alpha}$ gives a contribution to (18) lower than the contribution of the analogous terms with Δ_α and Δ_β by one order. The inclusion in (18) of the terms with $L_{\alpha\ldots\beta}$ and $L_{\beta\ldots\alpha}$ allows us to decide about the existence of surface waves and surface solitons in the case of the Langevin-type equations, as it has already been mentioned in Section 9.

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