Magnetic ordering of two-dimensional ion lattice and coherent states of delocalized charge carriers in this ion lattice

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Abstract. We have considered stable magnetic ordered structures on two-dimensional ion lattice with spins and states of delocalized charge carriers in these magnetic structures. These magnetic structures have short-range ferromagnetic order and long-range antiferromagnetic order. Besides magnetic momenta there are additional momenta with symmetry of the orbital momentum. Each of these inhomogeneous magnetic configurations is topologically stable and is characterized by their own field topological number \( q \) and a finite energy \( E_q \). As a result, these inhomogeneous configurations can exist at sufficiently high temperatures, for example, in classical (lanthanum, yttrium) high-temperature superconductors. These ion-field magnetic structures are not collapse because of interactions with current carriers. However, the charge carrier states are determined by structure of magnetic configurations. The energy functional of the charge carrier system is finite and single-valued only if the charge carrier system is coherent and has conserved momenta, whose symmetry is consistent with the structure of the ion-field configurations. We have found coherent charge carrier p-and d-states, and d-states have superconducting properties, but p-states can exist above the critical temperature \( T_c \).

1. Introduction
In our model the coherent states of charge carrier system are consequences of the existence of steady field configurations of ion lattice with special magnetic properties, in particular with short range magnetic order.

The study is carried out in two stages. At the first stage we consider ion-field stable configurations without delocalized electrons. Topological methods are used to establish conditions (the symmetry of fields and their distribution in space) of which the ion-field configurations are stable and have finite energy. The dynamical properties of ion-field system are described within field-theoretic approach.

At the second stage we examine the electron states in these ion-field stable configurations. The energy functional of charge carriers moving in the ion-field configuration is finite and single-valued only if the charge carrier system is coherent and has conserved momenta whose symmetry is coordinated with the structure of the ion-field configuration.

Since classical (lanthanum, yttrium) high-temperature (high-\( T_c \)) superconductors have quasi two-dimensional structure and magnetic properties the offered here model can be used for interpretation the charge carrier states in high-\( T_c \) superconductors.

2. The ion-field configurations with finite energy.
2.1.1. \textit{Geometry of the field problem.} We use the topological approach for finding stable ion-field configurations, which are not collapse in time owing to fluctuation and have a finite energy. Within the topological approach the stability of any configuration is determined by the geometry of the physical space and by the geometry of the internal space (the space of fields). The configurations are stable and have a finite energy if continuous maps (which will be determined below) of the physical space into the internal space are nontrivial.

In our task we have two-dimensional ion lattice. As we build continuous model, we abstract from a discrete lattice and consider two-dimensional plane instead of the ion lattice. We assume that the field value on the boundary of the physical space is the same (this corresponds to the Born-von-Karman boundary conditions), so in our task the two-dimensional plane is compactified into a two dimensional sphere $S^2_{\text{phys}}$. Thus, as the physical space we have two-dimensional sphere $S^2_{\text{phys}}$.

In each point of physical space the magnetic moment is a vector (is set by a vector). Each vector with the given direction defines a point on sphere $S^2$. The set of all available vectors forms sphere $S^2$. This sphere $S^2$ is accepted as internal space of the magnetic subsystem in our task.

By natural image it is possible to define the continuous maps of the physical space into the internal space. We designate it as $g$: $S^2_{\text{phys}} \to S^2$. From topology it is known, that these continuous maps are nontrivial and form the homotopy group $\pi_2(S^2)=\mathbb{Z}$, $q=1,2,3\ldots$ (group of integers).

So the system under consideration has global-space inhomogeneous ion-field configurations, each of that has own field topological number $q\in \pi_2(S^2)$, and a finite energy $E^q$.

The states of an ion lattice with the magnetic moments, which are non-uniform in space, traditionally are described using scalar fields associated with the three-parametric rotation group $SO(3)$ [1]. The elements of $SO(3)$ group form a three-dimensional projective space $RP^3$ (a three-dimensional sphere $S^3$ with identified opposite points, $RP^3=S^3/Z_2$, $Z_2$ is a cyclic group of two elements). The three-parameter $SO(3)$ group contains three scalar fields $\Phi^1$, $\Phi^2$ and $\Phi^3$. Two scalar fields $\Phi^1$ and $\Phi^2$ of the magnetic subsystem form two-dimensional sphere $S^2$, a subspace of the space $RP^3$ of the complete symmetry group.

As will be shown below, in addition to scalar fields, which were magnetization vectors in our case, the existence vector fields in a steady configuration are possible. The vector fields are caused with existence in examined structure of the additional moment, $\Phi^3$, which symmetry is distinct from symmetry of the magnetic momenta. These momenta have symmetry of the orbital momenta.

According to the Poincare theorem, always there are isolated singularity points of a vector field (special points, in which the vector field is equal to zero) on two-dimensional sphere, $S^2_{\text{phys}}$. At these special points the symmetry of scalar points may be broken. Outside these points there are two scalar fields, $\Phi^1$ and $\Phi^2$, but at these special points there are three scalar fields, $\Phi^1$, $\Phi^2$ and $\Phi^3$. So in the local region of isolated singularity points vector fields are generated. Indeed a point on the $S^2_{\text{phys}}$ can be surrounded by a contour mapped into a closed curve $S^1$ in the internal $RP^3$ space of scalar fields. Continuous maps $S^1 \to RP^3$ are specified by the homotopy group $\pi_1(RP^3)=Z_2$, where $Z_2$ is a cycle group consisting of two elements. One of these elements (the zero element) defines a trivial contour $S^1$ on $RP^3$, contacting to one point. But the other element defines a nontrivial contour not contacting continuously to a point.

A vector field in these isolated singularity points is zero, $A^\mu_\nu=0$. But in a vicinity of these points field is nonzero. The fields may be gauge in such a way that there remains only one nonzero angular component of the vector field, $A^\phi$. So the field configurations of such system characterized not only by the topological number $q\in \pi_2(S^2)$, which determines the contribution of the scalar fields, but also by the indices of the special points $q'\in \pi_1(RP^3)$, which determines the contribution of the vector fields.

Such scalar and vector field configurations are steady to perturbations and have a finite energy $E^q$.

2.2 Formalism. The energy states of field system. The $SO(3)$ group is the total group of symmetry of ion-field configurations. The scalar fields $\Phi(x)=\{\Phi^a(x), a=1,2, x=r,\phi\}$ take their values on the sphere $S^2$, a subspace of the space $RP^3$ of $SO(3)$ group. The vector fields $A_\mu(x)=\{A^\mu_\nu(x), a=1,2,3, \mu=\}$
\(r, \phi\) take on their values in the algebra of \(SO(3)\) group. Here \(\mu\) are indices of the physical space, and \(a\) are indices of the internal space, \(x\) is a coordinate of the physical space.

We study the space of fields for which the energy \(E_\Phi\) is finite and single-valued. Let the dynamics of scalar fields on the physical space be determined by the Lagrangian

\[
L_\Phi = \frac{1}{4} \sum_\mu \sum_a \left( \partial_\mu \phi^a(x) \right)^2 - \frac{1}{4} \lambda \left( \sum_a \phi^a(x) \cdot \phi^a(x) - C^2 \right)^2
\]

were \(\partial_\mu = \partial / \partial x^\mu\), \(\lambda\) is a positive constant, \(\lambda\) is a dimensional quantity, and \(C^2\) has the dimension of mass. Below we assume summation over repeated indices and drop the summation sing and internal-space indices.

The energy functional for the Lagrangian (1) is

\[
E_\Phi = \frac{1}{2} \int (\text{grad} \Phi(x))^2 d^2x + \frac{1}{4} \lambda \int \left( \Phi(x) \cdot \Phi(x) - C^2 \right)^2 d^2x.
\]

The finiteness of the last term on the right-hand side of eq. (2), \(\int_{-\infty}^{+\infty} \left( \Phi^2(x) - C^2 \right)^2 d^2x = \text{const}\) implies that \(\lim \Phi(x) = C\) as \(x \to \infty\). But then the second term on the right-hand side of eq. (2) is divergent, \(\int_{-\infty}^{+\infty} (\text{grad} \Phi(x))^2 d^2x \to \infty\).

However inclusion of vector fields allows to remove the divergence in the energy functional. The Lagrangian incorporated scalar and vector fields is

\[
L = L_G + \frac{1}{2} \left( D_\mu \Phi(x) \right) \left( D^\mu \Phi(x) \right) - \frac{1}{4} \lambda \left( \Phi(x) \cdot \Phi(x) - C^2 \right)^2,
\]

were \(L_G\) is a vector-field Lagrangian, and \(D_\mu\) is the covariant derivative,

\[
D_\mu \Phi(x) = \partial_\mu \Phi(x) + [A_\mu(x), \Phi(x)].
\]

The energy functional for the Lagrangian (3) is

\[
E_{\Phi,G} = E_G + \frac{1}{2} \int \left( D_\mu \Phi(x) \right) \left( D^\mu \Phi(x) \right) d^2x + \frac{1}{2} \lambda \int \left( \Phi(x) \cdot \Phi(x) - C^2 \right)^2 d^2x,
\]

were \(E_G = \frac{1}{2} \int F_{\mu\nu} F^{\mu\nu} d^2x\) is the contribution of field strength, \(F^{\mu\nu}_a\),

\[
F^{\mu\nu}_a = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu - [A^b_\mu, A^c_\nu].
\]

The two last terms in the energy functional (4) is finite if \(D_\mu \Phi(x) = 0\) and \(\lim \Phi(x) = C\) as \(x \to \infty\). Besides the energy functional (4) is minimal if

\[
D_\mu \Phi^a = e_{\beta\mu\nu} F^{\beta\mu\nu}.
\]

Formally the condition (5) resembles Bogomol’nyi’s condition [2], which minimizes the energy of a steady-state monopole. For examined system the condition (5) satisfies situations, when radial and temporary components of the vector fields are equal to zero, \(A_r = A_\phi = 0\) (a=1,2,3). But the angular component is nonzero, \(A_\theta = e f(r) \sigma_3\), were \(e\) is an unit vector directed at a tangent to a contour, covering a isolated singularity point of a vector field, \(f(r)\) coordinate function, \(\sigma_3\) is Pauli matrix.

In the limit \(\lambda \to 0\) the energy functional of scalar and vector fields (4) is finite and has the discrete spectrum of values \(E^q\), were \(q \in \pi(S)\). The energy has the lowest energy for \(q=1\).

3. Charge carrier states.

Since the stability of a field configuration is caused by topological reasons, it does not change because of interactions with charge carriers, i.e. the fields of stable configuration act as a thermostat for the
charge carrier system. The carriers moving in the ion fields can either receive energy from the fields or give it off to the fields without destroying of the ion-field configurations.

But the charge carrier states are determined the structure configuration. The energy functional of the charge carrier subsystem in the field configuration in term of a functional integral over all the histories of the field subsystem is

\[ E = \frac{1}{Z} \int DA^q \; D\Phi^q \, E\left(A^q, \Phi^q, \Psi\right) \exp\left(-i\hbar^{-1} S\left(A^q, \Phi^q, \Psi\right)\right), \quad (6) \]

were \( Z \) is the normalization constant, \( \Psi \) is the charge carrier wave function. The energy functional (6) is single-valued only if the part of the action of charge carrier subsystem, that is field-dependent, changes by an integral multiple of \( 2\pi \). Then the average energy of the entire charge carrier subsystem is single-valued and is characterized by the integer \( n \). This suggests that the charge carrier system in stable field configuration is characterized by quantum number and is coherent, i.e. charge carrier system has conserved momenta whose symmetry is coordinated with the structure of the ion-field configuration.

The angular momentum operator \( L \) that satisfies the gauge-invariant Hamiltonian of charge carrier system is

\[ H = (-1/2m)D^2 + V(r) \]

were \( D = \partial - ieA_\phi \) and a system of communication relations for the operator \( D \) and \( r \) has the form

\[ L = -[r, D] - qr |r|. \]

Then \( LL = -[r, D]^2 + q^2 \), and

\[ H = \frac{1}{2m} \left( \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) + \frac{l(l+1) - q^2}{2mr^2} + V(r), \quad (7) \]

were \( l(l+1) \) are the eigenvalues of the operator \( LL \). According to formula (7) for \( H \) the eigenvalue of the orbital angular momentum \( l \) is related to the field topological number \( q \): \( l=q, q+1, q+2, ... \)

For a moving charge carriers the orbital angular momentum \( L \) and spin momentum \( S \) are not conserved separately. But the total angular momentum \( J=L+S \) is conserved. The progection \( M \) of the angular momentum on the quantization axis is also conserved. Pair of eigenvalues \( j \) and \( m \) specified specifies the coherent state of charge carriers.

Thus, the \( p \)-state order parameter of charge carrier system \((l=1, s=1)\) with \( j=l \) and \( m=0 \) is defined by one vector \( z^k : B_{ij} = \delta_{ik} \cdot (z^k) \cdot \exp(i\phi) \). The \( d \)-state order parameter of charge carrier system \((l=2, s=0)\) consists of two vectors: \( z^k \) and \( y^k : B_{ij} = z_i (x_j + iy_j) + z_j (x_i + iy_i) \) for \( j=1, m=1 \).

The analysis of the boundary conditions shows that the coherent \( p \)-state of charge carrier system can exist only in the bulk medium. But the coherent \( d \)-state of charge carrier system can exists not only in the bulk medium but also at the medium boundary. In this \( d \)-state sustained translation charge carrier currents are generated. These currents have the properties of the superconducting current [3]. But coherent \( p \)-state has no superconducting properties. This \( p \)-state of charge carrier system can exists in a wide region of the phase diagram above the critical temperature \( T_c \) in the underdoped regime in high-\( T_c \) superconductors [4].

References
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