

TOPOLOGY OF MOMENTUM SPACE AND QUANTUM PHASE TRANSITIONS¹G.E. Volovik²*Low Temperature Laboratory, Helsinki University of Technology, P.O.Box 2200,
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Received 6 December 2005, in final form 9 January 2006, accepted 23 January 2006

Many quantum condensed-matter systems, and probably the quantum vacuum of our Universe, are strongly correlated and strongly interacting fermionic systems, which cannot be treated perturbatively. However, physics which emerges in the low-energy corner does not depend on the complicated details of the system and is relatively simple. It is determined by the nodes in the fermionic spectrum, which are protected by topology in momentum space (in some cases, in combination with the vacuum symmetry). Here we illustrate this universality on some examples of quantum phase transitions, which can occur between the vacua with the same symmetry but with different topology of nodes in momentum space.

PACS: 02.40.Pc, 67.57.z, 74.20.Rp, 73.43.Nq

1 Introduction

There are two schemes for the classification of states in condensed matter physics and relativistic quantum fields: classification by symmetry and by momentum space topology.

For the first classification method, a given state of the system is characterized by a symmetry group H which is a subgroup of the symmetry group G of the relevant physical laws. This classification reflects the phenomenon of spontaneously broken symmetry. In relativistic quantum fields the chain of successive phase transitions, in which the large symmetry group existing at high energy is reduced at low energy, is in the basis of the Grand Unification Theories (GUT) [1, 2]; that is why we can call this scheme the GUT scheme. In condensed matter, the spontaneous symmetry breaking is a typical phenomenon, and the thermodynamic states are also classified in terms of the subgroup H of the relevant group G (see e.g. the classification of superfluid and superconducting states in Refs. [3, 4]). The groups G and H are also responsible for topological defects, which are determined by the nontrivial elements of the homotopy groups $\pi_n(G/H)$; cf. Ref. [5].

The second classification method reflects the opposite tendency – the anti Grand Unification (anti-GUT) – when instead of the symmetry breaking the symmetry gradually emerges at low

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energy. This method deals with the ground states of the system at zero temperature ($T = 0$), i.e., it is the classification of quantum vacua. The universality classes of quantum vacua are determined by momentum-space topology, which is also responsible for the type of the emergent physical laws at low energy. For systems living in 3D space, there are four basic universality classes of fermionic vacua [6, 7]:

(i) Vacua with fully-gapped fermionic spectrum (such as conventional superconductors).

(ii) Vacua with fermionic excitations characterized by Fermi points – points in 3D momentum space at which the energy of fermionic quasiparticle vanishes. Examples are provided by superfluid $^3\text{He-A}$ and also by the quantum vacuum of Standard Model above the electroweak transition, where all elementary particles are chiral fermions. This universality class manifests the phenomenon of emergent relativistic quantum fields at low energy: close to the Fermi points the fermionic quasiparticles behave as massless Weyl fermions, while the collective modes of the vacuum interact with these fermions as gauge and gravitational fields.

(iii) Vacua with fermionic excitations characterized by lines in 3D momentum space or points in 2D momentum space. We call them Fermi lines, though in general it is better to characterize zeroes by co-dimension, which is the dimension of \mathbf{p} -space minus the dimension of the manifold of zeros. Lines in 3D momentum space and points in 2D momentum space have co-dimension 2, since $3 - 1 = 2 - 0 = 2$; compare this with zeroes of class (ii) which have co-dimension $3 - 0 = 3$. Fermi lines are topologically stable only if some special symmetry is obeyed. Example is provided by high T_c superconductors where the pairing into a d -wave state occurs.

(iv) Vacua with fermionic excitations characterized by Fermi surfaces. The representatives of this universality class are normal metals and normal liquid ^3He . This class manifests the phenomenon of emergent non-relativistic physics: at low temperature all the metals obey the Landau theory of Fermi liquid, which is based on the stability of Fermi surface. Fermi surface has co-dimension 1: in 3D systems it is the surface (co-dimension = $3 - 2 = 1$), in 2D systems it is the line (co-dimension = $2 - 1 = 1$), and in 1D systems it is the point (co-dimension = $1 - 0 = 1$; the Landau theory does not work here, but the Fermi surface survives).

The possibility of the Fermi band class (v), where the energy vanishes in the finite region of the 3D momentum space and thus zeroes have co-dimension 0, has been also discussed [8–11].

The phase transitions which we discuss here are quantum phase transitions (QPT) [12]. It may happen that by changing some parameter q of the system we transfer the vacuum state from one universality class to another with the same symmetry group H . The point q_c , where this zero-temperature transition occurs, marks the QPT. For $T \neq 0$, the phase transition is absent, as the two states belong to the same symmetry class H . Hence, there is an isolated singular point $(q_c, 0)$ in the (q, T) plane (see Fig. 1 in the extended version of this paper [13]).

The QPTs which occur in classes (iv) and (i) or between these classes are well known. In the class (iv) the corresponding quantum phase transition is known as Lifshitz transition [14], at which the Fermi surface changes its topology or emerges from the fully gapped state of class (i), see Sec. 2. The QPT between the fully gapped states with different topological charges occurs in 2D systems exhibiting the quantum Hall and spin-Hall effect: this is the plateau-plateau QPT between the states with different values of the Hall (or spin-Hall) conductance (see Sec. 5). The less known QPTs involve point nodes [15–19] (Sec. 3) and nodal lines [20, 21] (Sec. 4).

2 Fermi surface as topological object and Lifshitz transition

In ideal Fermi gases at zero temperature, the Fermi surface is the boundary in the momentum \mathbf{p} -space between the occupied states ($n_{\mathbf{p}} = 1$) and empty states ($n_{\mathbf{p}} = 0$). The spectrum of fermions is $E(\mathbf{p}) = p^2/2m - \mu$, where $\mu > 0$ is the chemical potential and m is the mass of a fermionic atom or electron. The Fermi surface at $p = p_F = \sqrt{2\mu m}$ separates the occupied negative energy states with $p^2/2m - \mu < 0$ from the empty positive energy states with $p^2/2m - \mu > 0$. At this boundary the energy of particles is zero, $E(\mathbf{p}) = 0$. What happens when the interaction between particles is introduced? Due to interaction the distribution function $n_{\mathbf{p}}$ is no longer exactly 1 or 0. However, the stability of the Fermi surface is protected by topology of the Green's function at imaginary frequency, $G^{-1} = i\omega - (p^2/2m) + \mu$.

Let us for simplicity skip one spatial dimension p_z so that the Fermi surface becomes the line in 2D momentum space (p_x, p_y) ; this does not change the co-dimension of zeroes which remains $1 = 2 - 1$. The Green's function has singularities lying on a closed line $\omega = 0, p_x^2 + p_y^2 = p_F^2$ in the 3D momentum-frequency space (ω, p_x, p_y) (see Fig. 2 in [13]). This is the line of the quantized vortex in the momentum space, since the phase Φ of the Green's function $G = |G|e^{i\Phi}$ changes by 2π around any path embracing any element of the vortex line. The winding number cannot change by continuous deformation of the Green's function: the momentum-space vortex is robust toward any perturbation. Thus the singularity of the Green function on the Fermi surface is preserved, even when interaction between fermions is introduced.

The Green function is generally a matrix with spin indices. In addition, it may have the band indices (in the case of electrons in the periodic potential of crystals). In such a case the phase of the Green function becomes meaningless; however, the stability of the Fermi surface is protected by the topological invariant describing the winding number of a vortex in (ω, \mathbf{p}) space:

$$N_1 = \text{tr} \oint_C \frac{dl}{2\pi i} G(\mu, \mathbf{p}) \partial_l G^{-1}(\mu, \mathbf{p}). \quad (1)$$

The integral is over contour C around a vortex; tr is the trace over spin, band or other indices.

There are two scenarios of how to destroy the vortex loop in momentum space: perturbative and non-perturbative. In the second scenario the non-perturbative reconstruction of the spectrum removes the Fermi surface, as it occurs at the superconducting transition when the gap appears.

The first scenario reproduces the process occurring for the loop of quantized vortex in superfluids and superconductors. The vortex ring can continuously shrink to a point and then disappear. This is allowed by topology, since the opposite elements of the vortex line have opposite winding numbers N_1 , which annihilate each other: $1 - 1 = 0$. In the momentum space this occurs when one continuously changes the chemical potential from the positive to the negative value: at $\mu < 0$ there is no vortex loop in momentum space and the vacuum is fully gapped. The point $\mu = 0$ marks the QPT – the Lifshitz transition – at which the topology of the energy spectrum changes. At this QPT the symmetry of the vacuum does not change. The other types of the Lifshitz transition are related to reconnection of the vortex lines in p -space (Fig. 3 in [13]).

3 Fermi point as topological object

The crucial non-perturbative reconstruction of the spectrum occurs at the superfluid transition to $^3\text{He-A}$, where the point nodes emerge instead of the Fermi surface. Let us consider the

Bogoliubov–Nambu Hamiltonian which qualitatively describes fermionic quasiparticles in this axial state of p -wave pairing [4]:

$$H = \begin{pmatrix} p^2/2m - \mu & c_{\perp} \mathbf{p} \cdot (\hat{\mathbf{e}}_1 + i \hat{\mathbf{e}}_2) \\ c_{\perp} \mathbf{p} \cdot (\hat{\mathbf{e}}_1 - i \hat{\mathbf{e}}_2) & -p^2/2m + \mu \end{pmatrix} = \tau_3(p^2/2m - \mu) + c_{\perp} \mathbf{p} \cdot (\tau_1 \hat{\mathbf{e}}_1 - \tau_2 \hat{\mathbf{e}}_2), \quad (2)$$

where τ_1, τ_2 and τ_3 are 2×2 matrices in Bogoliubov–Nambu particle-hole space (the spin structure is irrelevant for consideration). The orthonormal triad $(\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2, \hat{\mathbf{I}} \equiv \hat{\mathbf{e}}_1 \times \hat{\mathbf{e}}_2)$ characterizes the order parameter, with the unit vector $\hat{\mathbf{I}}$ showing the direction of the orbital momentum of the Cooper pair (or of the diatomic molecule in case of BEC); and c_{\perp} is the speed of the quasiparticles propagating in the plane perpendicular to $\hat{\mathbf{I}}$. The energy spectrum of fermions is

$$E^2(\mathbf{p}) = \left(\frac{p^2}{2m} - \mu \right)^2 + c_{\perp}^2 (\mathbf{p} \times \hat{\mathbf{I}})^2. \quad (3)$$

In the BCS regime occurring for positive chemical potential $\mu > 0$, there are two Fermi points (points where $E(\mathbf{p}) = 0$): at $\mathbf{p}_1 = p_F \hat{\mathbf{I}}$ and $\mathbf{p}_2 = -p_F \hat{\mathbf{I}}$ (Fig. 4 in [13]).

For a general system, be it relativistic or nonrelativistic, the topological stability of the Fermi point is guaranteed by the nontrivial homotopy group $\pi_2(GL(n, \mathbf{C})) = \mathbf{Z}$ which describes the mapping of a sphere S^2 embracing the point node to the space of non-degenerate complex matrices [7]. This is the group of integers. The integer valued topological invariant (winding number) can be written in terms of the fermionic propagator $G^{-1}(i\omega, \mathbf{p}) = i\omega - H(\mathbf{p})$ as a surface integral in the 4D frequency-momentum space $p_{\mu} = (\omega, \mathbf{p})$: [6]

$$N_3 \equiv \frac{1}{24\pi^2} \epsilon_{\mu\nu\rho\sigma} \text{tr} \oint_{\Sigma_a} dS^{\sigma} G \frac{\partial}{\partial p_{\mu}} G^{-1} G \frac{\partial}{\partial p_{\nu}} G^{-1} G \frac{\partial}{\partial p_{\rho}} G^{-1}. \quad (4)$$

Here Σ_a is a 3D surface around the isolated Fermi point $p_{\mu a} = (0, \mathbf{p}_a)$; the trace in is over the Bogoliubov-Nambu spin. The two Fermi points \mathbf{p}_1 and \mathbf{p}_2 have nonzero topological charges $N_3 = +1$ and $N_3 = -1$. Close to any of the Fermi points the energy spectrum of quasiparticles acquires the relativistic form. In particular, the spectrum in Eq.(3) becomes [6]:

$$E^2(\mathbf{p}) = g^{ik} (p_i - eA_i)(p_k - eA_k), \quad (5)$$

where the analog gauge field is $\mathbf{A} = p_F \hat{\mathbf{I}}$; the effective ‘‘electric charge’’ is either $e = +1$ or $e = -1$ depending on the Fermi point; and the effective metric is $g^{ik} = \text{diag}(c_{\perp}^2, c_{\perp}^2, c_{\parallel}^2 = p_F^2/m^2)$. The density of states (DoS) due to Fermi points is $\nu(E) \propto E^2$.

Let us consider an example of QPT governed by the \mathbf{p} -space topology: between a fully-gapped vacuum state and a vacuum state with topologically-protected point nodes [15, 16]. Such QPT may occur in a system of ultracold fermionic atoms in the region of the BEC–BCS crossover, provided Cooper pairing occurs in the non- s -wave channel (for elementary particle physics, such transitions are related to CPT violation, neutrino oscillations, and other phenomena [17]). The QPT occurs if one varies the chemical potential μ . For $\mu < 0$, Fermi points are absent and the spectrum is fully-gapped (Fig. 4 in [13]). In this topologically-stable fully-gapped vacuum, the density of states is drastically different from that in the topologically-stable gapless regime: $\nu(E) = 0$ for $E < |\mu|$. This demonstrates that the QPT under consideration

is of purely topological origin: it occurs when two Fermi points with $N_3 = +1$ and $N_3 = -1$ merge and form one topologically-trivial Fermi point with $N_3 = 0$, which disappears at $\mu < 0$. The intermediate state at $\mu = 0$ is marginal: the \mathbf{p} -space topology is trivial ($N_3 = 0$) and cannot protect the vacuum against decay into one of the two topologically-stable vacua unless there is a special symmetry which stabilizes the marginal node. Such symmetry protects Fermi points in the Standard Model above the electroweak phase transition [6].

4 Fermi lines

In general the zeroes of co-dimension 2 (nodal lines in 3D momentum space or point nodes in 2D momentum space) do not have the topological stability. However, if the Hamiltonian is restricted by some symmetry, the topological stability of these nodes is possible. The nodal lines do not appear in spin-triplet superconductors, but they may exist in spin-singlet superconductors [3, 22]. The analysis of topological stability of nodal lines in systems with real fermions was done by Horava [7].

An example of point nodes in 2D momentum space is provided by the layered quasi-2D high- T_c superconductor. In the simplest form, the relevant Hamiltonian is

$$H = \tau_3 \left(\frac{p_x^2 + p_y^2}{2m} - \mu \right) + a\tau_1(p_x^2 - \lambda p_y^2). \quad (6)$$

In case of tetragonal symmetry one has $\lambda = 1$, but in a more general case $\lambda \neq 1$ and the order parameter represents the combination of d -wave ($p_x^2 - p_y^2$) and s -wave ($p_x^2 + p_y^2$) components. At $\mu > 0$ and $\lambda > 0$, the energy spectrum $E^2(\mathbf{p}) = (p^2/2m - \mu)^2 + a^2(p_x^2 - \lambda p_y^2)^2$ contains 4 point nodes in 2D momentum space:

$$p_x^a = \pm p_F \sqrt{\frac{\lambda}{1 + \lambda}}, \quad p_y^a = \pm p_F \sqrt{\frac{1}{1 + \lambda}}, \quad p_F^2 = 2\mu m. \quad (7)$$

Do these nodes survive or not if we extend Eq.(6) to the more general Hamiltonian obeying the same symmetry? The important property of this Hamiltonian is that, as distinct from the Hamiltonian (2), it obeys the time reversal symmetry T which prohibits the imaginary τ_2 -term. In the spin singlet states the Hamiltonian obeying the T-symmetry must satisfy the equation $H^*(-\mathbf{p}) = H(\mathbf{p})$. The general form of the 2×2 Bogoliubov-Nambu spin-singlet Hamiltonian satisfying this equation can be expressed in terms of the 2D vector $\mathbf{m}(\mathbf{p}) = (m_x(\mathbf{p}), m_y(\mathbf{p}))$:

$$H = \tau_3 m_x(\mathbf{p}) + \tau_1 m_y(\mathbf{p}). \quad (8)$$

Using this vector one can construct the integer valued topological invariant – the contour integral around the point node in 2D momentum space (or around the nodal line in 3D momentum space):

$$N_2 = \frac{1}{2\pi} \oint dl \hat{\mathbf{z}} \cdot \left(\hat{\mathbf{m}} \times \frac{d\hat{\mathbf{m}}}{dl} \right), \quad (9)$$

where $\hat{\mathbf{m}} \equiv \mathbf{m}/|\mathbf{m}|$. This winding number of a point vortex in 2D space (p_x, p_y), which is robust to any change of the Hamiltonian respecting the T-symmetry, protects the node in the spectrum.

All four nodes in Eq.(6) are topologically stable, since nodes with equal signs ($++$ and $--$) have winding number $N_2 = +1$, while the other two nodes have winding number $N_2 = -1$ (Fig. 8 in [13]). To destroy the nodes one must either violate the T-symmetry or to deform the order parameter in such a way that the nodes merge and then annihilate each other forming the fully gapped state. This is what happens when one changes the asymmetry parameter λ . The point $\lambda = 0$ marks the QPT from gapless to the fully gapped spectrum (Fig. 8 in [13]).

Probably such a QPT has something to do with the unusual behavior observed in high- T_c cuprate $\text{Pr}_{2-x}\text{Ce}_x\text{CuO}_{4-\delta}$ [24]. It was found that the field dependence of electronic specific heat $C(T, H)$ is linear at $T=2\text{K}$, which is consistent with fully gapped state, and non-linear at $T \geq 3\text{K}$, which is consistent with existence of point nodes in 2D momentum space. This was interpreted in terms of the conventional phase transition with the change of symmetry from s -wave to d -wave when temperature is decreased. But the behavior of $C(T, H)$ is the consequence of the topology of the spectrum rather than of the symmetry. That is why it is more natural to identify the observed behavior with the QPT which is smeared due to finite temperature.

A similar QPT when μ crosses zero can occur in the BCS-BEC crossover region [20, 21].

5 Plateau transitions in fully gapped 2D systems

The fully gapped vacua in 2D systems or in quasi-2D thin films, though they do not have zeroes in the energy spectrum, can also be topologically non-trivial. They are characterized by the invariant obtained by dimensional reduction from the Fermi point topological invariant in Eq.(4):

$$\tilde{N}_3 = \frac{1}{24\pi^2} e_{\mu\nu\lambda} \text{tr} \int d^2 p d\omega G \partial_{p_\mu} G^{-1} G \partial_{p_\nu} G^{-1} G \partial_{p_\lambda} G^{-1} . \quad (10)$$

There is no singularity in the Green's function. The integral is either over the entire 3-momentum space $p_\mu = (\omega, p_x, p_y)$, or in a crystalline system it is bounded by the Brillouin zone.

An example is provided by the 2D version of the Hamiltonian (2) with $\hat{1} = \hat{z}$, $\hat{e}_1 = \hat{x}$, $\hat{e}_2 = \hat{y}$. Since now $p^2 = p_x^2 + p_y^2$, the quasiparticle energy (3) becomes

$$E^2(\mathbf{p}) = \left(\frac{p_x^2 + p_y^2}{2m} - \mu \right)^2 + c_\perp^2 (p_x^2 + p_y^2) . \quad (11)$$

It is nowhere zero. The Hamiltonian (2) can be written in terms of vector $\mathbf{g}(p_x, p_y)$:

$$\mathcal{H} = \tau^i g_i(\mathbf{p}) , \quad g_3 = \frac{p_x^2 + p_y^2}{2m} - \mu , \quad g_1 = c_\perp p_x , \quad g_2 = -c_\perp p_y . \quad (12)$$

The distribution of the unit vector $\hat{\mathbf{g}}(p_x, p_y) = \mathbf{g}/|\mathbf{g}|$ in the momentum space has the same structure as the skyrmion in real space (see Fig. 9 in [13]). The topological invariant for this momentum-space skyrmion is given by Eq.(10) written in terms of the unit vector $\hat{\mathbf{g}}(p_x, p_y)$:

$$\tilde{N}_3 = \frac{1}{4\pi} \int dp_x dp_y \hat{\mathbf{g}} \cdot \left(\frac{\partial \hat{\mathbf{g}}}{\partial p_x} \times \frac{\partial \hat{\mathbf{g}}}{\partial p_y} \right) . \quad (13)$$

Since at infinity the unit vector field $\hat{\mathbf{g}}$ has the same value, $\hat{\mathbf{g}}_{p \rightarrow \infty} \rightarrow (0, 0, 1)$, the 2-momentum space (p_x, p_y) becomes isomorphic to the compact S^2 sphere. The function $\hat{\mathbf{g}}(\mathbf{p})$ realizes the mapping of this S^2 sphere to the S^2 sphere of the unit vector $\hat{\mathbf{g}}$ with winding number \tilde{N}_3 .

This and other similar topological charges give rise to quantization of Hall and spin-Hall conductivities, which occurs without external magnetic field (the so-called intrinsic quantum Hall and spin quantum Hall effects). There are actually 4 responses to transverse forces which are quantized under appropriate conditions. These are: quantized response of the mass current (or electric current in electrically charged systems) to transverse gradient of chemical potential $\nabla\mu$ (transverse electric field \mathbf{E}); quantized response of the mass current (electric current) to transverse gradient of magnetic field interacting with Pauli spins; quantized response of the spin current to transverse gradient of magnetic field; and quantized response of the spin current to transverse gradient of chemical potential (electric field) [25]. All these can be described using the generalized Chern-Simons term [6]:

$$F_{\text{CS}}\{\mathbf{A}_Y\} = \frac{1}{16\pi} N_{IJ} e_{\mu\nu\lambda} \int d^2x dt A_\mu^I F_{\nu\lambda}^J, \quad (14)$$

where A_μ^I is the set of the gauge fields: in addition to the conventional electromagnetic potential A_μ one can introduce the auxiliary gauge fields. In particular, the auxiliary $SU(2)$ gauge field A_μ^a is convenient for the description of the spin-Hall effect, since the variation of the action with respect to A_μ^a gives the spin current: $\delta S/\delta A_\mu^a = J_a^\mu$. The prefactor N_{IJ} is expressed in terms of the topological invariant:

$$N_{IJ} = \frac{1}{24\pi^2} e_{\mu\nu\lambda} \text{tr} Q_I Q_J \int d^2p d\omega G \partial_{p_\mu} G^{-1} G \partial_{p_\nu} G^{-1} G \partial_{p_\lambda} G^{-1}, \quad (15)$$

where Q_I is the charge interacting with the gauge field A_μ^I . To obtain, for example, the response of the spin current j_x^z to the electric field E_x , one must consider two charges: the electric charge $Q_1 = e$ and the spin along z as another charge, $Q_2 = s_z = \hbar\sigma_z/2$. This gives the spin current response to the electric field $j_x^z = (N_{s_z e}/4\pi) E_x$, where $N_{s_z e}$ is $e\hbar/2$ times integer.

This consideration is applicable, when the momentum (or quasi-momentum in solids) are the well defined quantities, otherwise (for example, in the presence of impurities) one cannot construct the invariant in terms of the Green's function $G(\mathbf{p}, \omega)$. However, it is not excluded that in some cases the perturbative introduction of impurities does not change the prefactor N_{IJ} in the Chern-Simons term (14) and thus does not influence the quantization: this occurs if there is no spectral flow under the adiabatic introduction of impurities. In this case the quantization is determined by the reference system – the fully gapped system from which the considered system can be obtained by the continuous deformation without the spectral flow (analogous phenomenon for the angular momentum paradox in $^3\text{He-A}$ was discussed in [26]). The most recent review paper on the spin current can be found in [27].

The integer topological invariant of the ground state cannot follow the continuous parameters of the system. That is why when one changes such a parameter, for example, the thickness of the film, one finds a set of quantum phase transitions between different integer values of the invariants (Fig. 10 in [13]), and thus between the plateaus in Hall or spin-Hall conductivity.

6 Conclusion

Here we discussed the quantum phase transitions which occur between the vacuum states with the same symmetry above and below the transition. These transitions are essentially different

from conventional phase transitions accompanied by the symmetry breaking. The transitions considered here are purely topological – they are accompanied by the change of the topology of fermionic Green's function in \mathbf{p} -space without change in the vacuum symmetry. The \mathbf{p} -space topology, in turn, depends on the symmetry of the system. The interplay between symmetry and topology leads to variety of vacuum states and thus to variety of emergent physical laws at low energy, and to variety of possible quantum phase transitions. The more interesting situations are expected for spatially inhomogeneous systems, say for systems with topological defects in \mathbf{r} -space, where the \mathbf{p} -space topology, the \mathbf{r} -space topology, and symmetry are combined [28].

Acknowledgement: This work is supported in part by the Russian Ministry of Education and Science, through the Leading Scientific School grant #2338.2003.2, and by the European Science Foundation COSLAB Program.

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