Surface defects in vesicle aggregates and anyons

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We consider surface defects in connection to the closed vesicle form evolution in mesomorphism of lyotropic aggregates, based on the experimental data by Feigenson [1] on confocal fluorescent resonant microscopy for the lipid DPPC/DLPC/cholesterol system. To estimate the influence of surface topological defects onto aggregate form it has been used the fractional quantum Hall effect (FQHE) description [2, 3].

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1. Introduction. Topological methods are suitable for the description of surface and bulk defects [4, 5], and also for describing the shape evolution of lyotropic liquid crystal aggregates. Some types of surface defects of micelles and vesicles with closed surface have been predicted in frame of fluctuation-dissipation (FD) theorem and Goldstone theorem [6]. This studying stimulated by observed phenomena of surfaces of nanoscopic domains in lipid mixture dipalmitoylphosphatidylcholine/dilauroylphosphatidylcholine/cholesterol (DPPC/DLPC/cholesterol) [1] that have not topological interpretation. In Feigenson experiments [1] on lyotropic mesomorphism it was observed phase inhomogeneity at asymmetric shape of closed lipid vesicle, which also may be considered as n-axis gyration effects induced by the mixture component variation. Minimum surface domains diameter is on the order of 50 – 60Å and an island consist about 40-60 lipids in 1-phase regime (D-region at the phase diagram, Fig. 1, Fig. 2.) between the different cholesterol concentration.

The widespread description for phase behavior of fluid membranes is based on the Ginzburg-Landau (GL) free-energy functional. As well known, this functional with the same the order parameter describes the transitions in 1-type superconductors [7] and in superfluidity He - phases [2]. Moreover, the GL theory is exact in the symmetries of anyons [3].

2. Topology of vesicular closed aggregates. By studying the membrane organization properties, Park et. al. [2] have revealed that the free-energy of a closed membrane (spherical vesicle) is similar to the free-energy of a superconducting film [2, 7], and also to the free energy of a transversal quantum magnetic flux with a superconducting vortex flowing around (for the complex order parameter ψ).

ψ = ψ0 \prod_{i=1}^{2n} (\sin \frac{\theta}{2} \cos \frac{\theta_i}{2} \exp [i(\phi - \phi_i)/2] - \cos \frac{\theta}{2} \sin \frac{\theta_i}{2} \exp [-i(\phi - \phi_i)/2]) \equiv \psi_0 P(\Omega),

where Ω = (θ, φ). The order parameter ψ and the shape parameter of the vesicle ρ below the phase transition temperature is calculated by minimizing H over ψ0 and the zeros positions \{Ω\} of the function P(Ω). For instance, in the case n = 3 the polynomial P(Ω) contains 81 terms. Without writing the expressions [2] corresponding to the effective density of free energy as an expansion in Legendre polynomials, we recall that the shape functions corresponding to a figure of n-atic order are of the form ρ(Ω) = ψ02ρ(n)(Ω), that is, proportional to ψ02 ∼ r – r_c.

This generate set has exactly 2n zeros at arbitrary positions on the sphere and is equivalent in form to fractional wave functions for anyons [3].

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We can consider the quantum Hall wave functions, which describe particles with fractional charge \[ m = 3, 8 \]. The many-particle wave function is

\[ \Psi_N^{(m)} = \prod_{i<j} (u_i v_j - u_j v_i)^m, \] (2)

where \( m \) is relative angular momentum of a pair of particles, \( (2l - m) \) is total angular momentum, \( (u, v) = (\cos \frac{1}{2} \theta e^{i\phi/2}, \sin \frac{1}{2} \theta e^{-i\phi/2}) \) are spinor variables describing the particle coordinates. The numerical solution for three-particle wave function \( \Psi_N^{(m)} \) in spherical geometry was found in [3].

Taking into account the fluctuations effects, we will receive the qualitatively changed results about the spherical functions [2]. The relation between the vesicle shape and the evolution of surface defects could play a significant role.

2.1. One example: Helfrich hat model with fractional number of molecules. In the context of the membrane organization problems, Helfrich [9] considered fluctuations effects on membrane surfaces. In his construction (so called "hat model") he introduced the entropy term, dependent on the local curvature, which is induced by the thermal individual molecules motion, corresponding to de Broglie wavelengths. The entropy [5] is

\[ S_0 = -\frac{1}{2} k_B \ln (N + \ln (2\pi)) \] (3)

and corresponds to an effective number of hats given by

\[ N_j = \frac{J_j^2 (r) dA}{J_j^2 (r) |_{\text{max}} A}, \] (4)

however in entropy calculations this term plays the role of the particle number and it follows from [14], that is not an integer number in general. In the expression [4] \( r = (x, y) \) are vector coordinates, \( A \) is area under the hat, or the area occupied by a molecule. \( J_j \) is the mean curvature.

This phenomenological entropy presentation serves to clarification the physical reason of surface fluctuations, leading to the shape transformation of whole vesicle.

2.2. Vesicle symmetry and surface defects. Among the known types of topological defects (hedgehogs, boojums etc.) in case of the closed membrane we have observed only surface ones. If from the experimental data it is possible to restore distribution of the director field \( \mathbf{n} \), then it is possible to define the characteristics of defects [3], which in our case are convenient for classifying as linear surface features (boundaries of islands). They can be connected with the hedgehogs who have left on a surface. In any case of the defects displacement, the conservation law of a surface charge should be complied out [5].

![FIG. 1: Ternary phase diagram for DPPC/DLPC/cholesterol at 297K [1]. Where A, DLPC-rich fluid lamellar phase; B, coexisting fluid lamellar phase and DPPC-rich ordered phase; C, DPPC-rich ordered phase; D, a single phase that changes continuously from rigid ordered phase at the C/D boundary to a fluid-ordered phase at the D/E boundary; E, a fluid-ordered phase; F, a fluid-ordered phase different from E; G, coexisting crystalline cholesterol monohydrate and a cholesterol-saturated lamellar phase.](image)

Taking into account the Gauss-Bonnet formula, for the islands boundaries we know the expression [1]:

\[ \frac{1}{2\pi} d\theta + \int w (1 \times \frac{d\mathbf{w}}{ds}) ds = m - \frac{1}{2\pi} \int u K dS = m - \chi (\partial u), \] (5)

where \( \partial u \) is the domain boundary, \( \theta \) is angle at going round the domain boundary, \( w \) is vortex vector, \( \mathbf{w}(1 \times \frac{d\mathbf{w}}{ds}) = k_g \) is geodesic curvature and \( m \) is algebraic sum of dotty vortexes circulation quanta in a domain \( u \). The surface topology depends on the Euler characteristics \( \chi \) and influence upon total vortexes number [4].

At the vesicle surface, the topological vortexes (with genus 0) are directed both clockwise and counterclockwise. Their number is increasing in accordance to the vesicle sizes growth. The linear vortexes are the boundaries of the surface islands. The number of islands are always more, than one, when the simplex corresponds to topologically regular partition [4]. In this case the next equality take place: \( E_+ - E_- = \chi (M^2) - 2N \), here \( N \) is a number of surface islands, \( E_+ - \) the number of positive and negative directional simplex of partition \( M^2 \), as shown, it is whole here and should correspond to the condensate with whole statistics.

At the spherical bilayer membrane, it is possible to observe two types of regions: three-particles domains (consisting the disordered mixture DPPC/DLPC/cholesterol, these components are labelling three different kinds of molecules) and one-particle islands (with only lipids). Their common topo-
logical charge should be the same at any lyotropic transformations. Looking onto the evolution of surface domains [1], it is possible to surmise, that the Euler characteristic become closed to two, but nonequal it.

As may seem at first sight, at finite membrane thickness, displacement and deformation of any defects are forbidden at all. However, if the observed vesicle transformation, as expected [1], is the continuous phase transition, then the molecules of lipids come out from the volume always and they supplement into the composition of the membrane or leave it.

The director field has a normal surface term, causing to outlet of the hedgehogs to the surface. Topologically regular partition no longer corresponds to the physical meaning of surface domains, the Euler characteristic should be fractional.

The Laughlin wave functions of FQHE have not translational invariance [3], but they are describing a circular droplet of fluid, which must be confined in an external potential.

In [8] for spherical geometry, the states with the different defects combination, which correspond to Bose, Fermi and fractional statistics, are described. But in thermodynamical limit on a sphere, the particles of whole statistics stay only [10]. (Although there are manifolds (a torus [10]), where the particles of fractional statistics described by multicomponent wave functions, are existing.)

Our membrane consist of the molecules of two amphiphilic monolayers, whose tails are turned towards each other and heads are directed toward the disordered phase inside and outside of the bilayer sphere.

In our case of manifolds on two concentric spheres ($M_1 = S^2_1$ and $M_2 = S^2_2$), both are connected by the value of the closed membrane thickness, which is defined due to the lipid conformation. The order parameters $\psi_1 = \langle \exp[in\theta_1] \rangle$ and $\psi_2 = \langle \exp[in\theta_2] \rangle$ are different, just as spinor variables $(u_1, v_1) = (\cos \frac{1}{2} \theta_1 e^{i\phi_1/2}, \sin \frac{1}{2} \theta_1 e^{-i\phi_1/2})$ and for the second sphere index, respectively. This fact of the connected state of the closed spherical monolayers is an unproved hypothesis, but which is permitted to explain the fractal axes and the asymmetric vesicle shape.

3. Concluding remark. Thus, in light of FQHE description, the each molecule of the same kind of lyotropic mixture may be formally equivalent to anyon. Using a numerical simulation with the statistical Monte Carlo algorithms, it will be possible to define the type of observed phase transitions in actual and to calculate the structural domain sizes suitable to the axes geometry evolution.

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