Phase transitions in membranes with high genus

E. I. Kats [1,2], M.Monastyrsky [3]

May 30, 2012

1 Preface

In our paper we discuss some geometrical ideas to determine phase transitions in complex liquid membranes. Such membranes exist in many physical media.It is worthwhile to note that the description of phase transition in liquid membranes represents from the physical point of view far reaching generalization of the theory of holes introduced by Yakov Frenkel as early 1920's [2].

Beside the great physical interest their study leads to highly nontrivial mathematical problems,concerning with the very new fields of geometry and topology.

2 Introduction.

The membranes that we shall consider here are thin and flexible sheets of amphiphilic molecules. Such a construction distinguishes this object from similar systems like liquid interfaces or shells. On the interface of liquids the exchange of particles between both volume phases occurs. It corresponds to finite surface tension $\approx 100\ erg/sm^2$. For membranes which are in equilibrium with the solvent of amphiphilic molecules the number of molecules is fixed. That means zero surface tension. So, the energy of membranes is characterized mainly by bending energy but not by a surface tension. For liquid membranes which we are discussing the characteristic bending module is of the order of temperature, $\kappa \simeq 10^{-14}$ erg. This is the principal distinction with shells where characteristic bending energy is of the order 10^{11} erg, 25 orders higher than in the case of liquid membranes. So, for membranes we must use statistical mechanics approach , whereas for shells we apply elasticity theory. In solvents lipids or surfactants bilayers typically form closed surfaces or vesicles. The characteristic length scale of vesicle is of order $1-10\ \mu m$. There are a diversity of forms of membranes[3, 4]. Better known membranes with simple topology like sphere and torus but in experiments one observed membranes with higher genuses, e.g. with $g = 2, 3$ [5, 6]. Here g is the number of handles.

There exist also non-compact membranes like a stack of layers which posses cylindrical or plane geometry. Such super-molecular aggregates can be self-organized on a large scales and exhibit phases with different types of orientational and translational order.

For example spherical vesicles can be organized in three-dimensional cubic lattice, or infinite cylinders can be packed in two-dimensional hexagonal lattice. Let us mention that in this case, crystalline order exists on large scales (in typical examples of order 10^{-4} cm, whereas on the smaller scales the system remains liquid. There exist also other structures builded by infinite layers. The simplest example is the one-dimensional lattice of almost plane layers. Such a structure L_α called laminar is the analogy of smectic liquid crystal. There exists also the phase Q_α with a space cubic symmetry and the bloc structure generated by infinite periodic surface of complicated topology. Schematically such structure can be determined in thermodynamic limit $g \to \infty$, as a three-dimensional cubic set of "handles". This structure is principally different from a topologically trivial cubic lattice of spherical vesicles. The melting process of periodically distributed phase Q_α leads to the isotropic phase,so called sponge phase L_3. The structural bloc of the phase Q_α is non-periodic minimal surface with finite density of handles g, however the space distribution of g is determined by the nearest order. In our talk we consider the new method of classification of different types of membranes and their phase transitions.

3 Willmore surfaces and Minimal surfaces in S^3

Here we discuss some mathematics which we use to describe phase transitions in membranes.

Let M^2 be a surface (closed, with boundary or non-compact) embedded in R^3.

Definition 1 *A surface M^2 is called Willmore surface if it is an extremum of the Helfrich-Willmore (HW) functional:*

$$F = \int_{M^2} H^2 \, dA \tag{1}$$

where H is the mean curvature, and dA is an area element.

By Gauss-Bonnet theorem (HW) functional is equivalent to the:

$$F = \int_{M^2} (k_1^2 + k_2^2) \, dA$$

where k_1 and k_2 are the principal curvatures of M and

$$H = \frac{k_1 + k_2}{2}$$

Therefore the extremum of functional (1) determine the most plane surfaces of fixed topology. The following result due to J.Weiner [7] is important for future use.

Proposition 1.

Let M^2 be a minimal surface in S^3 and γ is a stereographic projection $S^3 \to R^3$. Then

$$\gamma(\hat{M}^2) = M^2 \qquad \text{and} \qquad F(M^2) = \sigma(\hat{M}^2) \tag{2}$$

where $\sigma(\hat{M}^2)$ is the area of the minimal surface. This statement is valid both for closed surfaces and for the one with a boundary. Willmore surfaces are not exhausted by the projection of minimal surfaces. For example, there exist an infinite set of Willmore torus which are not equivalent to minimal torus in S^3 [8]. These torus are extremum of (1) but not a minima. This result, apparently, is true for a surfaces of a higher genus. Willmore surfaces of higher genus generated by minimal surfaces in S^3 were constructed in [9, 10]. It is important to emphasize that Willmore surfaces embedded in R^3 satisfied the following:

$$\int_{M^2} H^2 \, dA \geq 4\pi n$$

where n is the number of intersection points (n–different pre-images under projection). From this and the square estimation of minimal surfaces embedded in S^3 follows that all Willmore surfaces for $g \geq 2$ have at least points of intersections [1]

---

[1] The equivalence between the special Willmore surfaces and minimal surfaces following from the Proposition 2 leads to a deep analogy with the string theory. Minimal surfaces $M^2 \subset S^3$ are the "world sheets" of the string determined in S^3 with Nambu-Goto action.

4 Phase transitions with a change of membranes' topology

In the previous section we have shown that Willmore surfaces providing minimum of Helfrich energy in the fixed topological class $g = const$ are related to minimal surfaces and provide the minima of functional F. Therefore instead of calculating the partition function of the Hamiltonian (1) we are able to calculate the partition function determined by Gibbs factor $e^{-\int \sigma(\hat{M}^2) d\hat{A}}$ for minimal surfaces in S^3. Such approach is especially useful to determine the structures of complex topology, like cubic or sponge phases.Both of these structures are the phases with finite density of handles. In terminology of minimal surfaces in S^3 such structures according (2) relate to minimal surfaces with finite density of holes. Before going to more detailed discussion of this correspondence, let us add some words with respect to physical properties of cubic and sponge phase.

Cubic phase of complex liquids are constructed by triple-periodic surfaces. Elementary cell of such a structure of the scale of 10 μm to 150 μm consists of a large number of molecules which diffuse freely along the membrane. In this case cubic structure determined by periodic distribution of mass density $\rho(r)$ and other characteristics, including $g(r)$ related with this one. The sponge phase L_3 is determined by the short-range order of distribution $\rho(r)$ or $g(r)$. In the language of a dual system distribution of holes in S^3 we can speak about periodic in cubic case or amorphous in sponge phase distribution of holes density $n(r)$.

If the energy E_h of the hole creation in minimal surfaces is finite, then

---

The surfaces M^2 play the role of instantons in the Yang-Mills theory determined in the space S^3.

the mean density of holes can be estimated by

$$n \approx \frac{1}{\xi^2} \exp\left(-\frac{E_h}{T}\right) \tag{3}$$

where ξ^2 is the mean size of an elementary cell creating by the holes on a minimal surface. This size is related with the mean value of physical cell of a cubic structure by transformation (2). The exponential factor in Formula (3) has the meaning of the probability of creation of a hole. To estimate ξ we use the following observation. Let us write full (HW) functional (1) with the Gaussian curvature term:

$$F = \frac{\kappa}{2} \int H^2 \, dA + \bar{\kappa} \int K \, dA \tag{4}$$

where two bending modules κ and $\bar{\kappa}$ (saddle-splay) which determine a deformation of the membranes with respect to the mean and the Gaussian curvature correspondingly. The creation of a sponge and a cubic phases depends of a spontaneous rise of a complexity of the topology of the surface, that is a creation of handles or of passages between a layers. It happens when $\bar{\kappa} > 0$ since according Gauss-Bonnet theorem the second summand in (4) is equal $4\pi\bar{\kappa}(1 - N_h)$, where N_h is the number of handles. The process of a spontaneous creation of the handles leads to an appearing of an increasing number of handles, but of a smaller size. The process stops at the equilibrium scale ξ which we search. It happens when when the positive terms of higher order of the mean curvature will be equal with the negative term of the Gaussian curvature. For finding ξ we might estimate the summands of order H^{-4} and K^{-2} in the expansion (4). Minimization of the energy developed in such a way, determine the equilibrium scale ξ

$$\xi \simeq \sqrt{\frac{\kappa}{\bar{\kappa}}} a$$

We used the natural estimate κa^2 (a the molecular size) for the fourth order elasticity moduli.

It is important to point out that minimal surface on S^3 has a surface tension. The energy determined by the functional (2) proportional to the area and the coefficient of proportionality has the sense of the surface tension. Therefore, the interaction between the holes will be short-ranged instead of real membranes where due to the absence of a surface tension in the HW functional this interaction is long-ranged. The natural parameter for the estimation of an energy is its temperature. If R is a radius of the interaction then for the holes of the distances less than R, the energy of the interaction $U \sim T$. It is possible to neglect the interaction on the large distances. We can formalize that was said above by considering the following formula for free energy of the system of holes on the minimal surface in S^3.

$$F_h = Tn \ln \frac{n}{en_0} - Tn \ln(1 - n\xi^2) \tag{5}$$

here n is the density of holes. The first term in (5) determine the free energy of the ideal gas of holes and the second one determines an increase of a free energy related with the interaction creating by the nearest holes. We use (5) to describe a transition from a dilute phase of the holes to the dense liquid phase. Let us recall that a creation of holes on a minimal surfaces in S^3 corresponds to an increase the genus of a real membrane. Therefore, the dilute phase of holes can be assumed as a laminar phase L_α of membranes with rare passages between layers. The liquid holes phase simulates a sponge phase L_3. To determine of the order distribution of holes on the minimal surface (cubic phases generated by physical membranes) we have to add a summand in (5) depending not only on the holes mean density but also of their distribution on the minimal surface. In the mean field theory we infer one particle distribution function of holes displacement $\mathbf{u}$ with respect to their equilibrium positions:

$$\rho(\mathbf{u}) = \frac{1}{Z} \exp\left[-\frac{1}{2T} \sum_q \varepsilon(q)\, |\mathbf{u}(q)|^2\right]$$

where $\varepsilon(q)$ is the deformation energy of the holes distributions and

$$Z = \int D\mathbf{u}(q) \exp\left[-\frac{1}{2T}\sum_q \varepsilon(q)\ |\mathbf{u}(q)|^2\right]$$

The energy $\varepsilon(q)$ has the following expansion:

$$\varepsilon(q) = \tau_{\text{eff}} + \sigma_{\text{eff}}\ q^2 \tag{6}$$

where the term τ_{eff} is determined by the condensation energy of dense phase and the deformation energy is related with surface tension σ_{eff}. We can find the mean squared displacement

$$\left\langle |\mathbf{u}^2| \right\rangle = \frac{T}{\sigma_{\text{eff}}\sqrt{\tau_{\text{eff}}}}$$

and applying classical Lindemann melting criterion [11] for crystals obtain:

$$\frac{T}{\sigma_{\text{eff}}\sqrt{\tau_{\text{eff}}}} \simeq 0.1\ \xi^2$$

This determines the melting temperature of crystal of holes on a minimal surface or, according to our principle of equivalence of minimal surfaces and real membranes, the temperature of phase transition between cubic and sponge phase.

$$T \approx\simeq 0.1\ \xi^2\ \sigma_{\text{eff}}\sqrt{\tau_{\text{eff}}}$$

Let us mentioned that such a phase transition (ordering of holes on minimal surfaces or handles on Willmore surfaces) does not need a substantial alteration of the mean density. Therefore, it might be considered as a weak first order transition, so called weak crystallization phase transition [12].

Let us recall that the characteristics of a minimal surface in S^3, effective surface tension σ_{eff} and effective energy of holes condensation are related with physical characteristics of a real membrane in a very sophisticated manner. Some restrictions follow by the very possibility of creation of stable holes in S^3; it is easy to see e.g. that for $\sigma_{eff} = const$, i.e σ_{eff} is independent of of the shape and distribution of holes the creation of holes is impossible.

5 Conformal modes of membranes and vesicles

Let us discuss the properties of conformal symmetry for HW functional. Namely, conformal modes of the HW–functional determine anomalous strong conformal fluctuation of membranes.

A. The main property of HW functional is its invariance with respect to conformal transformations of an ambient space. The following statement due to G.Tomsen was proved in the 20th years of the XX century.

Proposition 2

Let M^2 be a Willmore surface and $M^2 R^3$ is a smooth embedding. The HW functional is invariant under the conformal group $G(R^3)$. The group $G(R^3)$, according to the classical Liouville theorem is generated by dilatation,rotations, translations and inversion. The group $G(R^3)$ is isomorphic to $O(4,1)$. It follows from the Proposition 2. that the number of geometrically nontrivial parameters of $G(R^3)$ that is not changing the shape of a surface is equal 4. To estimate the whole number of independent conformal modes of the HW functional we need to add some restrictions imposed by physical conditions. The liquid inside the vesicle is incompressible. So we get

$$V = const$$

Amphiphilic molecules are densely packed on a surface. Therefore

$$A = const$$

Using these properties it is not difficult to determine conformal modes and the related conformal diffusion.

B. The general case

Let us remind that the number of conformally nonequivalent compact surfaces is determined by the genus of a surface

$$\begin{cases} dim_R\, M_g^2 = 6g - 6 & \text{for } g \geq 2 \\ dim_R\, M_g^2 = 2 & \text{for } g = 1 \\ dim_R\, M_g^2 = 0 & \text{for } g = 0 \end{cases} \tag{7}$$

Comparing (7) with Liuoville theorem we obtain the number of conformal mode as $6g - 10$ for $g \geq 2$.

C. Minimal Willmore surfaces.

The answer for Willmore surfaces obtained by projection of minimal surfaces is substantially different. First of all the conditions 6. and 7. now are not independent. The estimation of moduli parameters of Willmore surfaces also needs more sophisticated technique.In the compact case we use the arguments of paper [13].

Let us denote the Moduli space of Willmore surfaces M_g^2 as $\mathcal{M}$.

1. Each surface M_g^2 posses a conformal metric and quadratic holomorphic differential $\omega = Q(z)dz^2$. For any ω there exists conformal metrics which determines a surface minimally embedded into S^3. The dimension of the moduli space of such surfaces is equal to $12g - 12$. It follows from the estimation of the space of differentials ω which is $6g - 6$ and the dimension of moduli space of Riemann surfaces which is also $6g - 6$. The number of different embedding of M_g^2 is determined by the number of different spinor structure on M_g^2. More precisely, if ϕ_1 and ϕ_2 are a different solutions of the Gauss–Weingarten equations for M_g^2 with the same ω and equal determinants $\det \phi_1 = \det \phi_2$ then they determine the same spinor structure on M_g^2. Let us choose on the space M_g^2 a basis of homological cycles a_i, b_i $(i = 1, ..., g)$ corresponding to the canonical cuts on M_g^2. The spinor structure is determined

by the monodromy transformation of solutions ϕ_i

$$\phi_i \to (-1)^{\alpha_{i+1}} \phi_i$$
$$\phi_i \to (-1)^{\beta_{i+1}} \phi_i$$

where $\alpha_i, \beta_i \in \{0, 1\}$.

The numbers (α_i, β_i), $\alpha = (\alpha_i, ..., \alpha_g)$, $\beta = (\beta_i, ..., \beta_g)$ are called the θ–characteristics of M_g^2. The θ–characteristics depend on the choice of basis in M_g^2. The invariant is the parity

$$[\alpha_i, \beta_i] = \sum_{i=1}^{g} \alpha_i \, \beta_i$$

Due to the parity it is possible to classify embedding of surfaces up to a regular homotopy. U.Pincal has shown that two surfaces are equivalent via a smooth homotopy if the parities of their θ characteristics coincide [14].

Using this result it is easy to estimate the number of conditions L which determine one valued embedding of a surface M_g^2. The monodromy representation is the mapping of the fundamental group $\pi_1(M_g^2) \to SU(2)$. The number L is determined by the triviality of monodromy along an arbitrary cycle c. The group $\pi_1(M_g^2)$ is determined by $2g$ generators with one relation, and taking into an account the motion along each cycle which is generated by conformal group $SL(2, C)$ we obtain $6(2g-1)$ real conditions. Let us add the general global transformation of S^3 so we obtain $12g - 12$ conditions. In this way we have shown that the number of equations and the number of parameters which determine compact minimal surfaces coincide. Apparently,the number of such surfaces is finite[2]. Well known examples of such surfaces were founded by Lawson [9] and Karcher, Pinkal and Sterling [10].

5. Spectral properties.

---

[2] It follows from our consideration that toric minimal surfaces does not have conformal diffusion modes.

Most of characteristics of membranes can be determined, for example, by the distribution of marked atoms or the temperature on the surface. This problem reduces to the to the determination of the spectra of the Beltrami-Laplace operator Δ on a surface. A determination of the shape and other geometrical characteristics of surface of a constant Gauss curvature by the spectra of Δ is the classical mathematical problem.For example, from the spectra it is possible to reconstruct,in a compact case, the volume,genus and length of closed geodesics. Moreover, in this case it is possible to prove that the number of surfaces with the same spectra are finite. In our case Willmore surfaces are determined by the equation

$$\Delta H + H(H^2 - K) = 0$$

and not need to be a surfaces with constant Gauss curvature.However,as we mentioned above, apparently the number of different compact minimal surfaces in S^3 is finite and so the problem of restoring Willmore surfaces from the spectra of its Laplacian is accessible.

Acknowledgements.

This research was partially supported by the grants RFBR 10-01-00463a.

References

[1] M.Marinov, J.of Nuclear Phys.,**28**, 251 (1978).

[2] J.Frenkel, Z.Phys, **35**, 652 (1926).See also Collected works **3**, (Acad. of Scinces of the USSR, Moscow, 1959).

[3] D.Nelson, T.Pvian, and S.Weinberg, Statistical Mechanics of Membranes and Surfaces (World Scientific, New York, 1989).

[4] G. Porte, J. Phys. Cond. Matter, **4**, 8649 (1992).

[5] B. Fourcade, M.Mutz, and D.Bensimon, Phys. Rev. Lett., **68**, 2251 (1992); E.I.Kats, V.V.Lebedev, JETP Lett., **61**, 57 (1995).

[6] F. Julicher, U.Seifert, and R.Lipowski, Phys. Rev. Lett., **71**, 452 (1993).

[7] J.L. Weiner, Indiana Univ. Math. J., **27**, 19 (1978).

[8] U. Pinkal, Invent. Math., **81**, 379 (1985).

[9] H.B. Lawson, Ann. Math., **92**, 335 (1970).

[10] H. Karcher, U.Pinkal, I.Sterling, J.Diff. Geom., **28**, 169 (1988).

[11] L.D.Landau, E.M.Lifshits, Statistical Physics, Part 1 (Pergamon, Oxford, 1980).

[12] E.I.Kats, V.V.Lebedev, A.R.Muratov, Phys. Repts, **228**, 1 (1993).

[13] A.I. Bobenko UMN, **46**, 3 (1991).

[14] U. Pinkal, Topology, **24**, 421 (1985).

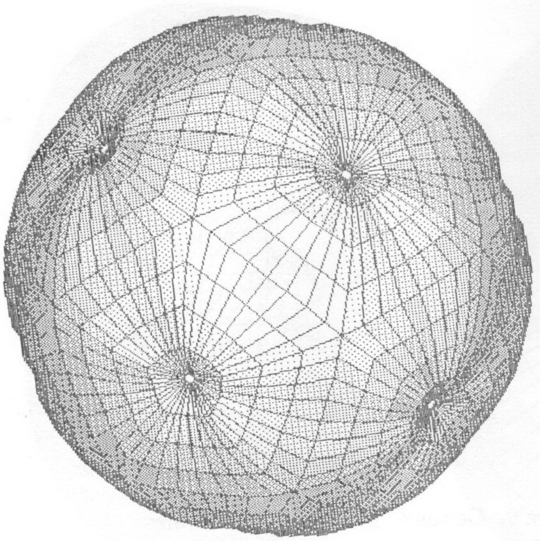


Figure 12. Genus 11, two dodecahedral bones.

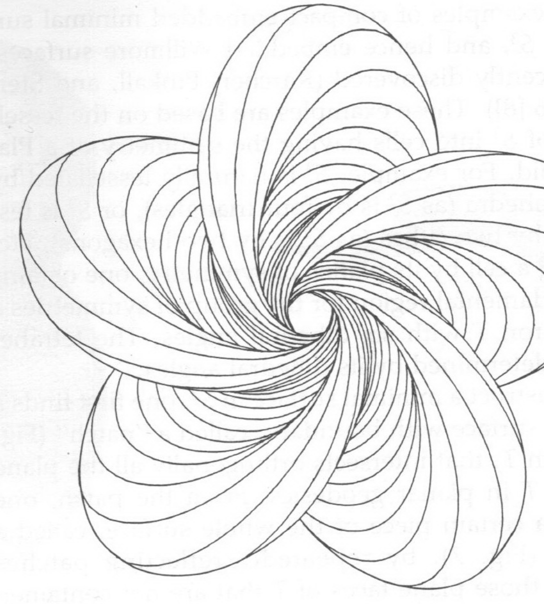


Figure 15.

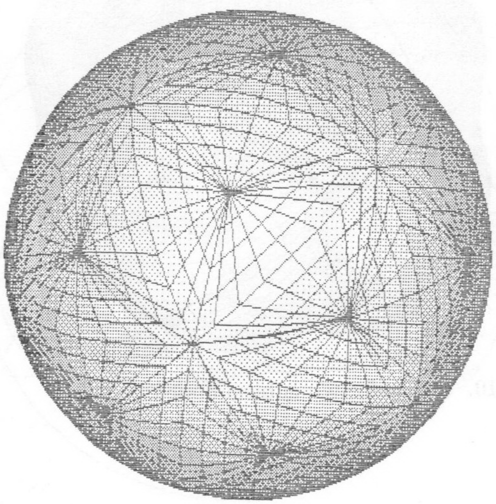


Figure 13. Genus 19, two icosahedral bones.

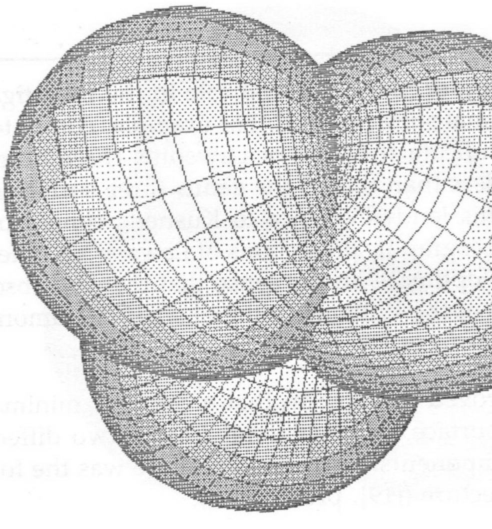
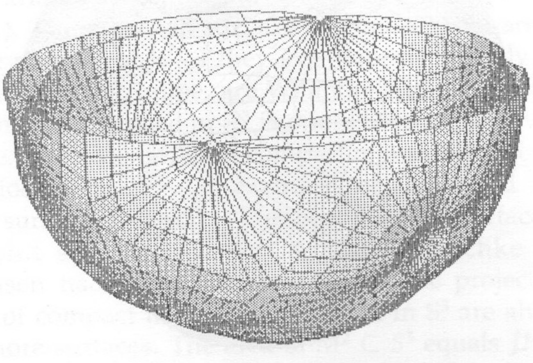
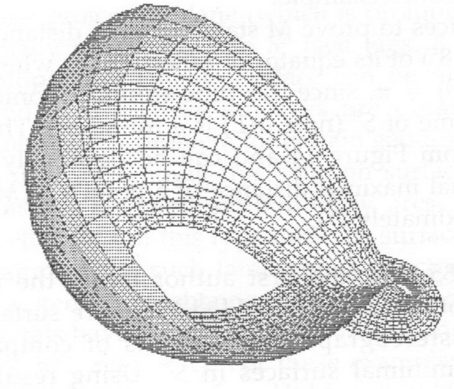
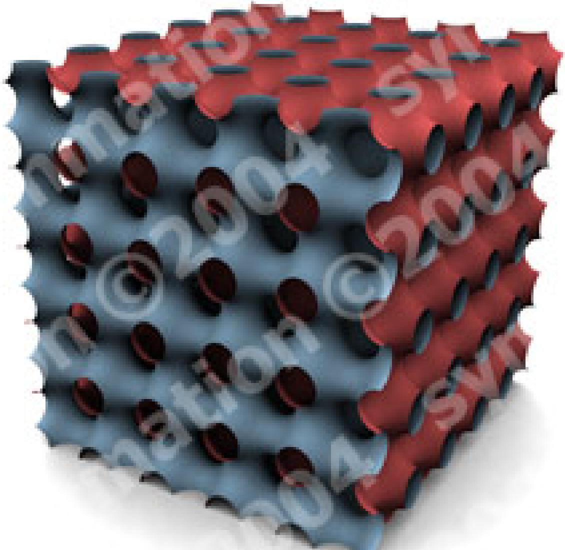
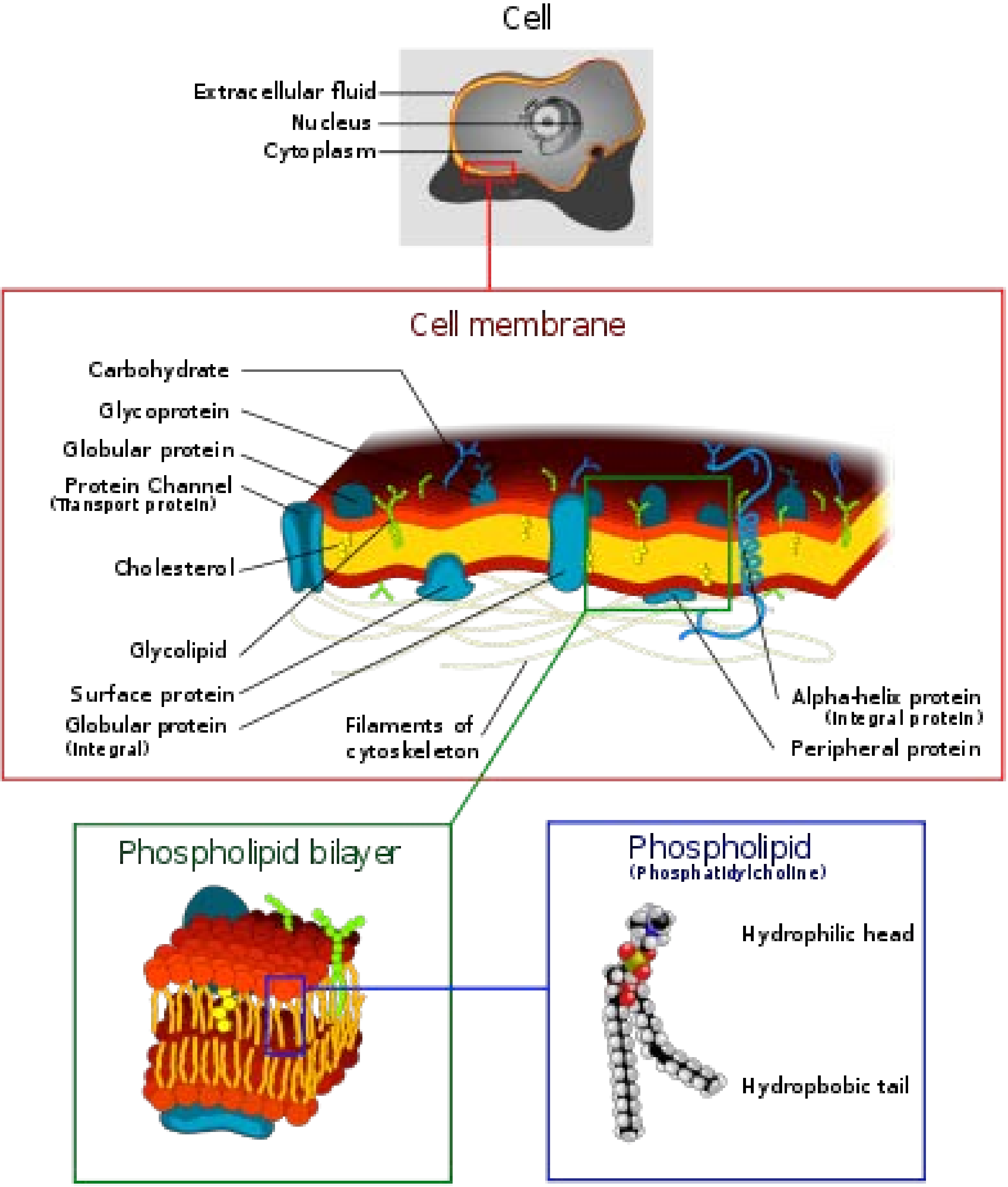


Figure 16.








Cell
Extracellular fluid
Nucleus
Cytoplasm
Cell membrane
Carbohydrate
Glycoprotein
Globular protein
Protein Channel
(Transport protein)
Cholesterol
Glycolipid
Surface protein
Globular protein
(integral)
Filaments of
cytoskeleton
Alpha-helix protein
(integral protein)
Peripheral protein
Phospholipid bilayer
Phospholipid
(Phosphatidylcholine)
Hydrophilic head
Hydropbobic tail