

Microscopic description of thermodynamics of Lipid Membrane at Liquid-Gel Phase Transition

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Over the years main phase transition in lipid membrane has been treated with various theoretical approaches, such as phenomenological [1], semi-empirical [2], and a number of microscopic approaches [3–5]. Some of the microscopic approaches resort to numerical methods [4, 5], though so far obtained results differ substantially from experiment [3]. Hence, consistent and comprehensive analytical description of the main phase transition is still missing. This paper is aimed to close this gap by considering consistently lipid molecules steric repulsion, van der Waals (VdW) attraction, and hydrophobic tension at the membrane water interface. The novelty of our approach is application of path-integral technique for description of steric repulsion between hydrocarbon chains.

Liquid to gel phase transition, referred to as “main phase transition” in literature, is first-order phase transition [6, 7] characterized by higher ordering of the lipid tails [8], a reduction of area per lipid and increase in membrane thickness [8, 9], a growth by an order of magnitude of membrane rigidity [10], a drop in self-diffusion coefficient [11], and change of volume per lipid [12]. Recently, main phase transition has been a topic of several molecular dynamics studies [8, 13]. Though, for most lipids a corresponding single-component lipid membrane undergoes this transition at a temperature significantly lower than the room temperature, an important exceptions exist for lipids with fully saturated hydrophobic chains, e.g., DMPC²⁾ ($T_m = 24^\circ\text{C}$) and DPPC ($T_m = 41^\circ\text{C}$). Moreover, a number of recent studies suggest that cholesterol might induce gel phase in lipid membrane [14, 15].

Present study belongs to a new stream of works caused by the recent increase of interest to the mem-

brane thermodynamics in a view of its role in the functioning of proteins [16–19].

In this paper we consider microscopic model and present a theory that makes transparent the physical mechanism of the liquid-gel phase transition. Our calculation results, obtained in a single approach, describe corresponding changes in the various thermodynamic characteristics, as well as dependence of main transition temperature on chain length. Though molecular dynamics studies [8, 13] achieved quantitative agreement with experiment in each particular case, they serve rather as numerical experimental tool complementing generalized physical concept of the underlying mechanisms clarified by the theory. In particular, it is clear that area per lipid in a gel phase is defined by the steric repulsion and van der Waals attraction, where as area per lipid in a liquid phase is defined by steric repulsion and hydrophobic tension. This is due to the degrees in which van der Waals attraction and hydrophobic tension depend on the area per lipid.

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²⁾DMPC stands for 1,2-dimyristoyl-sn-glycero-3-phosphocholine, DPPC stands for 1,2-dipalmitoyl-sn-glycero-3-phosphocholine

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