1 Introduction

Model lipid membranes present a gel-fluid transition usually called the main transition [1]. In the case of disassociating lipid, the main transition may be broadened and smoothed, depending on chain length and salt concentration. These effects may be observed by light scattering and other techniques [2]. We propose a generalization of the statistical model for neutral lipids proposed in [3] to include the effect of charge. In our model the lipid’s polar head may undergo dissociation, and a short-range (screened) electrostatic interaction favors the fluid phase, due to the larger distance between the headgroups. Simulations will be carried out using the Monte Carlo method. Results will be compared with mean field and experimental data.

2 Experimental Data

Experimental data for this project has been taken from [2], with authorization. Experiments using light scattering and reduced conductivity measurements all show difference in the behavior between dissociating and neutral lipids. The underlying reason for these differences has not been well established.

3 Statistical Model

Here we represent a mono-layer of the dissociating lipid on a square lattice, Ising-like model. We allow the lipids to be in four states, charged fluid, neutral fluid, charged gel or neutral gel. This is a generalization of the model proposed in [3] to include charge effects. The fluid/gel state with charges $q = 0$ or $q = 1$ variables, and the neutral/charged states with the $q = 0$ or $q = 1$ variables. See figure 3. The fluid states are degenerate, due to the high entropy of the disordered chain. The salt concentration is represented by the chemical potential $\mu$ for ions.

4 Mean Field Solution

The mean field solution for a simplified set of parameters has been carried out [4]. The resulting phase diagram is shown in figure 4.

5 Phase Transitions

For detection of the main order-disorder phase transition, we may simply measure the number of chains in the fluid phase (fig 6). The chosen function for this is

$$\Phi_1 = \frac{\sum_i \eta_i - 2\mu}{\phi}$$

where $\phi$ is the volume of the lattice. With this definition, if $\Phi_1$ is equal to $-1$ all lipids are in the gel state, and if $\Phi_1$ equals 1 all the lipids are in the fluid phase. In figure 5 we see a measurement of $\Phi_1$ in the phase transition region.

6 References