

Simulating Biological Membranes

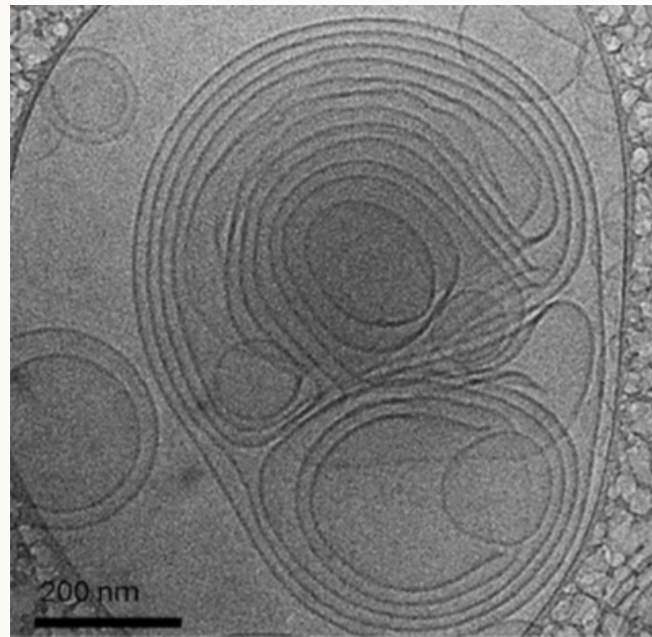
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Introduction

Biological membranes consist of so-called lipid-bilayers. That is double sheets of lipid molecules arranged back-to-back. Such layers make up the membranes enclosing living cells. They can also be found stacked on top of each other in the chloroplasts of plants, human lungs and electric eels. Stacked lipid-bilayers are of great interest in drug-delivery, photonics and biosensors. [1]



Lipids come in 2 varieties; saturated and unsaturated, or A and B for short. If the temperature in the layer is low enough, the lipids will tend to group together into continuous domains of A and B. Furthermore, what Tayebi et al found was that stacked layers will align themselves. That is, each layer will try and match its A/B domains with the one above and below, forming columns throughout the layers – a liquid crystalline structure.

Following the work of Hoshino et al, we have simulated stacked lipid-bilayers using the Ising model.

The Ising Model

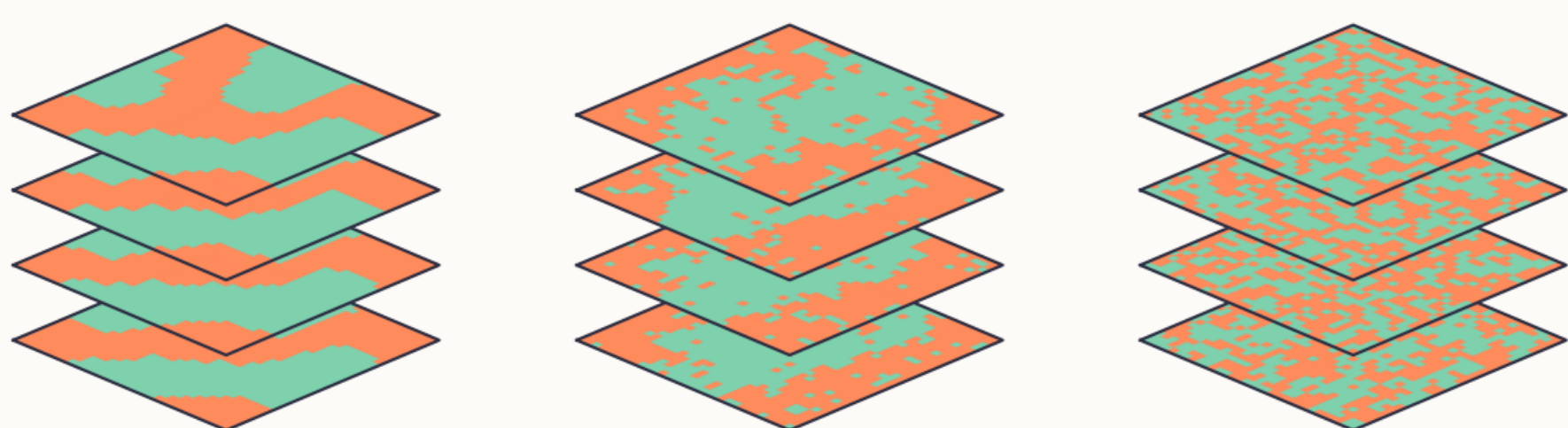
The Ising model was originally used to model magnetism. It consists of a discrete 3d grid of spin sites that can equal either +1 or -1, called a lattice. In our case, the lattice represents a stack of L_z bilayers of size $L \times L$, and $s_{i,\rho} = \pm 1$ represents lipid A/B filling the xy-position ρ in layer i . The energy of the lattice

$$H = -J \sum_{i, \langle \rho, \rho' \rangle} s_{i,\rho} s_{i,\rho'} - J_z \sum_{i, \rho} s_{i,\rho} s_{i+1,\rho},$$

where J, J_z are coupling constants and $\langle \rho, \rho' \rangle$ are any neighboring sites in a given layer. The first term accounts for intralayer interaction, the second for interlayer interaction.

Monte Carlo Simulation

By the Boltzmann distribution, any lattice state with energy E has a probability $p \propto e^{-E/T}$, where T is the temperature (and $k_B = 1$). To sample this distribution, we use the Monte Carlo method: First we find two random neighbors in a layer. Then we calculate the change in energy ΔE that an exchange of spins (A and B switching places) would cause. By exchanging according to the probability $p = e^{-\Delta E/T}$, we can converge towards a likely state given a random starting lattice. For a $32 \times 32 \times 8$ lattice like we have used, two random neighbors could be found more than 10^{10} times before the lattice stabilizes at a given energy.



$T/J = 1.0$

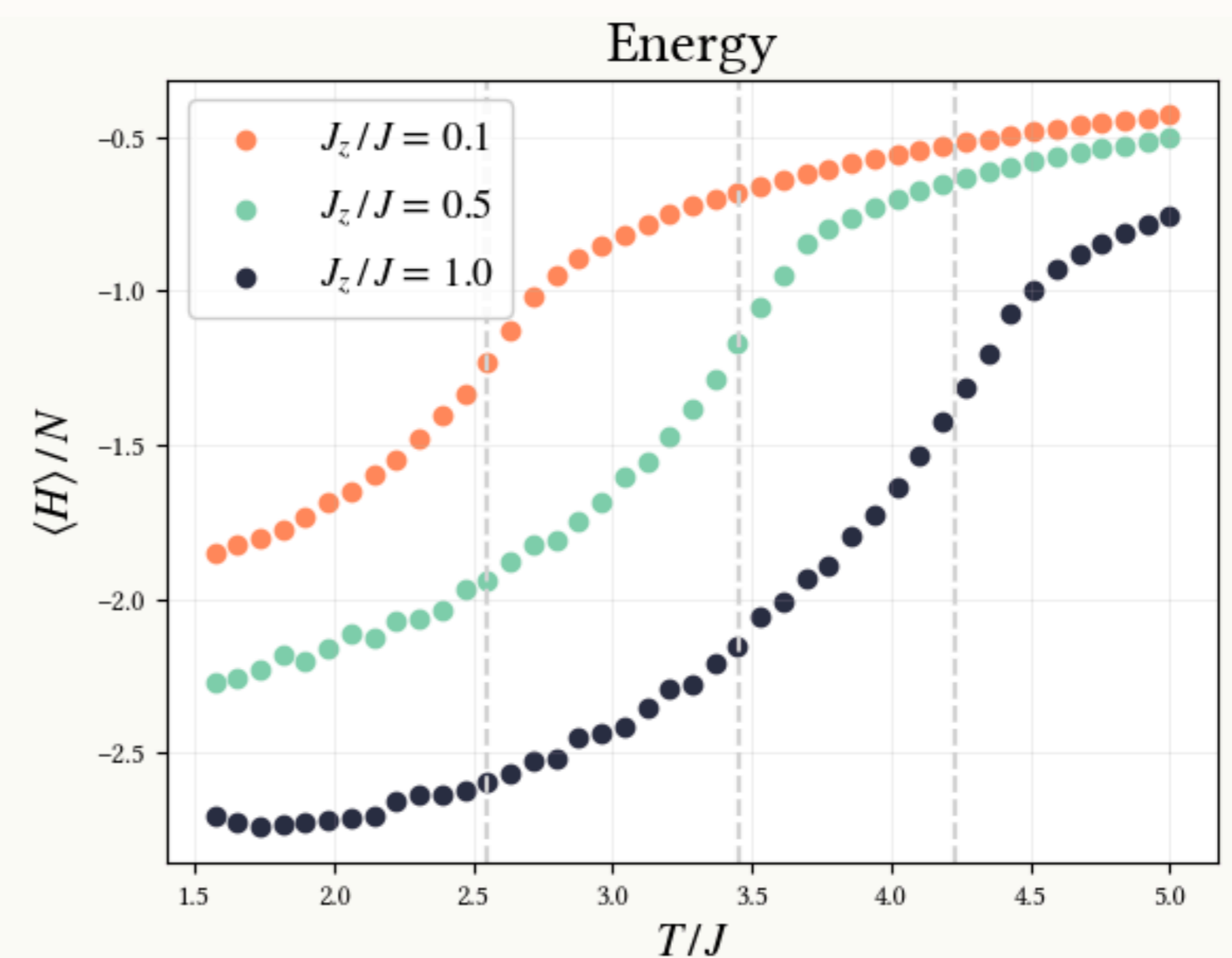
$T/J = 3.0$

$T/J = 6.0$

We see a phase transition from orderly and aligned lattices to disorder as the temperature increases.

Critical Temperature

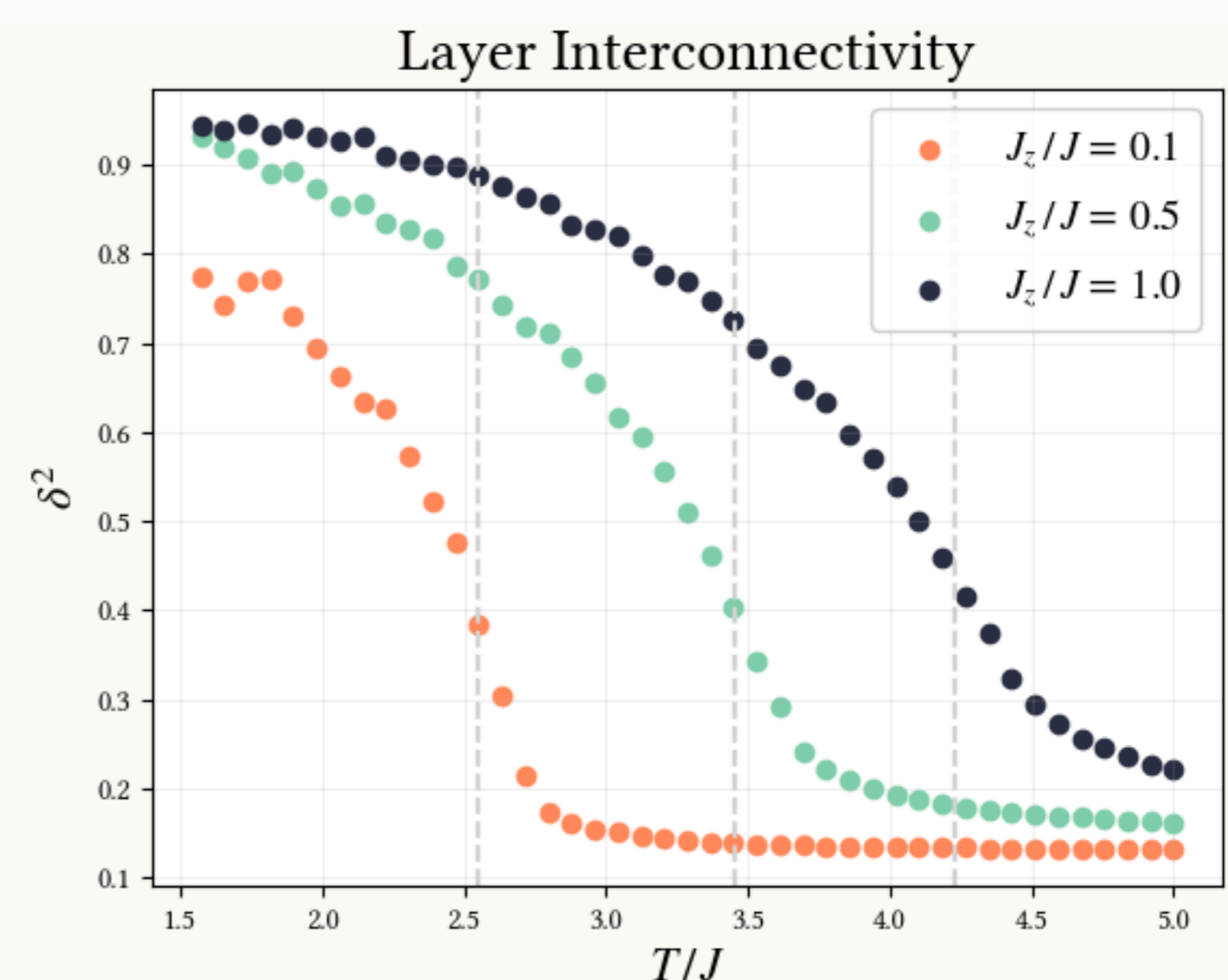
To identify where the lattice transitions from an orderly phase to a disorderly phase, we introduce the critical temperature T_c as the inflection point of the energy.



Above is the energy H averaged over an ensemble of equilibrated lattices (with $N = L^2 L_z$). Dashed lines show the critical temperature T_c .

Layer Interconnectivity

It is the columns of lipid A or B across the layers that allow transport of various chemicals through the membrane. To investigate this interconnectivity, we define $\delta^2 = (LL_z)^{-2} \sum_{\rho} \left(\sum_i s_{i,\rho} \right)^2$.



Above is δ^2 averaged over an ensemble of equilibrated lattices. Dashed lines show the critical temperature T_c , which line up with the inflection point of δ^2 , confirming a phase transition.

References

- [1] Tayebi et al. (2012) *Long-range interlayer alignment of intralayer domains in stacked lipid bilayers*. doi: 10.1038/nmat3451
- [2] Hoshino et al. (2021) *Correlated lateral phase separations in stacks of lipid membranes*. doi: 10.1063/1.4934984

The picture of a multilamellar vesicle is taken from de Barros et al. (2025). doi: 10.3390/pharmaceutics17111493

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