Free Energy Increment of Multilayer Membrane System due to Membrane-Membrane Interaction Potentials

Takao Yamamoto[1] and Kazunori Shimoda[2]
[1]Department of Physics, Faculty of Engineering, Gunma University, Kiryu, Gunma, 376-8515, Japan
[2]Department of Biological and Chemical Engineering, Faculty of Engineering, Gunma University, Kiryu, Gunma, 376-8515, Japan

Let us consider the statistical-mechanical model for fluid bilayer lipid membrane system expressed by the Hamiltonian,[1]

$$H(\{u_j(x,y)\}_{j,(x,y)}) = \sum_{j=1}^{n} H_{\rm one}(\{u_j(x,y)\}) + \sum_{i<j} \int {\rm d}x{\rm d}y V(u_j(x,y) - u_i(x,y)), \quad (1)$$

where the x-y plane is chosen to be parallel to the mean membrane plane, $z = u_j(x,y)$ is the shape of the j-th membrane ($j = 1, 2, \cdots, n$, K is the rigidity of the membrane, $V(z)$ is the membrane-membrane interaction potential and $\nabla = (\partial/\partial x, \partial/\partial y)$. Let the n-layer membrane system be embedded in an $L \times L \times L$ space. The partition function and the free energy per unit volume $f(\rho)$ ($\rho = n/L$ being the density of the membrane) are respectively given by[1,2]

$$Z = \int_{u_j<u_{j+1}} \prod_j \prod_{(x,y)} {\rm d}u_j(x,y) {\rm e}^{-\beta H}, \quad (2)$$

$$f(\rho) = -\frac{k_{\rm B}T}{L^3} \ln Z, \quad (3)$$

where $u_j < u_{j+1}$ denotes the non-crossing nature of the membrane and $\beta = 1/(k_{\rm B}T)$ ($k_{\rm B}$ being the Boltzmann constant and T being the temperature).

The free energy increment due to the membrane-membrane interaction potential V is given by $\Delta f(\rho) = f(\rho) - f_0(\rho)$, where $f_0(\rho)$ is the free energy for the $V = 0$ system (the "pure" non-crossing membrane system).

We proposed an approximate expression for the free energy increment,[3]

$$\Delta f(\rho) \simeq -k_{\rm B}T\rho \ln[\int_0^\infty {\rm d}s \exp(-\beta V(s)) P_0(s)], \quad (4)$$

based on the membrane-membrane distance distribution function;

$$P_0(s) =< \delta(u_{j+1}(x,y) - u_j(x,y)) >_{V=0}, \quad (5)$$

where $< \cdots >_{V=0}$ denotes the thermal average for the pure non-crossing membrane system. Using $P_0(s)$, we have an approximate expression:

$$\Delta f(\rho) \simeq -k_{\rm B}T\rho \ln[\int_0^\infty {\rm d}s \exp(-\beta V(s)) P_0(s)]. \quad (6)$$

From the results of the Monte-Carlo calculation based on the solid-on-solid membrane model[2,3], we have $P_0(s) = C_0\rho^3 s^2 \exp(-C_1\rho^2 s^2)$,where C_0 and C_1 are constants. Then, we obtain

$$\Delta f(\rho) = k\rho^4 + \mathcal{O}(\rho^5), \quad (7)$$

where k is a posive constant for the repulsive membrane-membrane interactions and a negative constant for the attractive interactions.

We peformed a Monte Carlo analysis to verify the above free nenergy increment expression for the membrane systems with the electrostatic repulsive potential and/or the van der Waals interaction potential. In Fig.1, the internal energy incremet per membrane unit area, $\Delta\epsilon(\rho) = -\rho^{-1}T^2\partial(\Delta f/T)/\partial T$, for the electrostatic potential system ($k_{\rm B}T = 2.6J$, J being the "microscopic" rigidity[2])is shown. The streight line is expressed by $\Delta\epsilon(\rho) = 0.0000746 - 12.0\rho^3 \simeq -12.0\rho^3$. Note that the "lattice space" is chosen as the length unit in this result. These results strongly support the ρ^4 behavior (7) of the free energy increment.

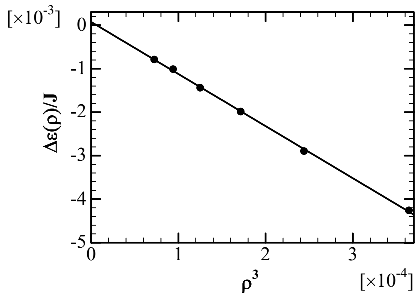

Figure 1: Internal energy increment.

References

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