Effect of Nonlinear Curvature Stiffness upon Fluctuation Pressure between Membranes

H. Kleinert

Institut für Theorie der Elementarteilchen

Freie Universität Berlin

Arnimallee 14

D-1000 Berlin 33

ABSTRACT

We calculate the repulsive pressure between planar membranes on top of each other at the one loop level in the presence of the full non-linear curvature stiffness. For short distances, smaller than the de Gennes persistence length, the pressure shows Helfrich's $1/d^3$ law with logarithmic corrections. In the opposite limit, it crosses over to the exponential falloff exp $[-2\pi(d/d_0)^2]$ where d_0 is a length scale characterizing the interpenetrability of the membranes.

Work supported in part by Deutsche Forschungsgemeinschaft under grant Kl 256.

Some time ago it was observed by Helfrich[1] that the most important force to keep membranes apart against the attraction of van der Waals forces is the entropic pressure caused by thermal undulations. The van der Waals forces decrease at distances smaller than the membrane thickness like $1/d^3$. For much shorter distances there are also hydration and electrostatic effects. For larger distances, the power of falloff increases and reaches $1/d^5$ at around 1000Å. In the vacuum, retardation effects change this to $1/d^6$.

By considering a membrane with the bending energy

$$E = \frac{1}{2\alpha} \int d^2\xi \ (\partial^2 u)^2 \tag{1}$$

(where $u(\xi)$, $\xi=(\xi^1, \xi^2)$ are the vertical displacements of the membrane). Helfrich, found an undulation pressure

$$p = c\, T^2 \alpha / d^3 \tag{2a}$$

with an unknown proportionality constant c, on whose size he could give various order of magnitude estimates. In recent Monte-Carlo simulations, it was measured to be[2]

$$c \approx 0.1 \tag{2b}$$

It is obvious that the simple law (2) will receive corrections due to the non-linear nature of the curvature energy ($u_i \equiv \partial_i u$)

$$E = \frac{1}{2\alpha} \int d^2\xi \sqrt{1+u_i^2}\ [\partial_i (u_i/\sqrt{1+u_i^2}\,)]^2 \tag{2c}$$

The renormalization of the non-linear inheractions necessitates the introduction of a mass scale Λ, the inverse molecular size, and this combines with the stiffness, α^{-1}, to form a non-perturbative length scale

$$\zeta \approx \Lambda^{-1} e^{4\pi/\alpha} \tag{3}$$

called the de Gennes persitence length, which sets the scale over which the membrane follows effectively the energy (1). Beyond this scale, the energy is effectively $(\partial^2 u) + \zeta^{-2} (\partial u)^2$. When going from $\xi \ll \zeta$ to $\xi \gg \zeta$ the correlation functions of the tangent vectors $\partial_i u$ change from an algebraic to an exponential falloff.

We therefore expect the $1/d^3$ law to be valid only for $d \ll \zeta$ and go over to an exponential falloff for $d \gg \zeta$. The purpose of this note is to show precisely how this happens.

Let us first give a convenient simple derivation of the $1/d^3$ law which can easily be extended by the non-linear curvature effects. We consider two membranes u_1 and u_2 which follow the energy (1).

$$E_0 = \frac{1}{2\alpha} \int d^2\xi \, [(\partial^2 u_1)^2 + (\partial^2 u_2)^2] \tag{4}$$

The condition that they impede each others undulation is imposed by a Lagrange multiplyer γ, adding to (4) the term

$$E_\gamma = \frac{\gamma}{4\alpha} \int d^2\xi \, [(u_1 - u_2 - d)^2 - \varepsilon_1 d^2] \tag{5}$$

It acts to maintain, on the average, a local distance d between the membranes with a Gaussian distribution of width $1/\sqrt{\varepsilon_1}$ around the average position. The parameter ε_1 measures the interpenetrability of the membranes.

By adding E_0+E_γ and integrating out the u fluctuations we find, after a quadratic completion, the free energy density.

$$f = \frac{T}{2}\int[d^2k/(2\pi)^2]\ \left\{\ln(G^{-1}(k)) - \frac{\gamma^2 d^2}{4\alpha^2}\left[(1,-1)\,G(k)\begin{pmatrix}1\\-1\end{pmatrix}\right]_{k\to 0} - \frac{\gamma}{4\alpha}\varepsilon_1 d^2\right\} \tag{6}$$

where $G^{-1}(k) \equiv \begin{pmatrix}A & B\\ B & A\end{pmatrix}$ with $A = k^4 + \frac{\gamma}{2}$, $B = -\frac{\gamma}{2}$.

Hence the last two terms combine to $-(\gamma/4\alpha)\,\varepsilon\, d^2$ with $\varepsilon = 1+\varepsilon_1$. The integral over k can be done after subtracting the system without distance constraint (i.e., $\gamma=0$) and we find

$$f = T\sqrt{\gamma}/8 - \frac{\gamma}{4\alpha}\varepsilon d^2 \tag{7}$$

Since γ is a Lagrange multiplyer, (7) has to be maximized in γ which gives

$$\sqrt{\gamma_m} = \frac{T}{4}\frac{\alpha}{\varepsilon d^2} \tag{8}$$

with an energy

$$f_m = T\frac{\sqrt{\gamma_m}}{16} = \frac{T^2}{64}\frac{\alpha}{\varepsilon d^2} \tag{9}$$

and a pressure

$$p = -\frac{\partial f_m}{\partial d} = \frac{T^2}{8}\frac{\alpha}{\varepsilon d^3} \tag{10}$$

just as in (2a).

Consider now the effect of the non-linear energy (2c). We go to the conformal parametrization of the surface $\underset{\sim}{x}(\xi)$ in which the metric is diagonal, $g_{ij}=\partial_i \underset{\sim}{x} \partial_j x = \rho\delta_{ij}$ and enforce this condition via

$$E_1 = \frac{1}{2\alpha} \int d^2\xi \, [\rho \, (\frac{1}{\rho} \, \partial \underset{\sim}{x})^2 + \lambda^{ij} \, (\delta_{ij} \, \partial_i \underset{\sim}{x} \, \partial_j \underset{\sim}{x} \, - \rho\delta_{ij})] \tag{11}$$

In a one-loop approximation, we shall assume ρ to lie at an extremum, which by symmetry is constant over the membrane. Also, $\lambda^{ij}=\lambda\delta_{ij}$. Assuming a flat background configuration $x^{1,2}{}_0(\xi)=\xi^{1,2}$ and introducing the intrinsic momenta $q=k/\sqrt{\rho}$ we integrate out the vertical undulations and find the free energy density

$$f_1 = \rho \left\{\frac{T}{2} \int \frac{d^2q}{(2\pi)^2} \ln (k^4+\lambda k^2) - \frac{\lambda}{\alpha} + \frac{\lambda}{\alpha\rho})\right\}$$

$$= \rho \left\{\frac{T}{2} \frac{\lambda}{4\pi} \, [\ln (\Lambda^2/\lambda)-1] - \frac{\lambda}{\alpha} + \frac{\lambda}{\alpha\rho} \right\} \tag{12}$$

Here is the place to introduce a dimensionally transmuted coupling constant

$$(\bar{\lambda})^{1/2} \equiv \Lambda^1 \, \exp\left\{-\frac{8\pi}{T\alpha}\right\} \tag{13}$$

In terms of $\bar{\lambda}$, the free energy takes the simple form

$$f_1 = \rho \left\{ \frac{T}{2} \frac{\lambda}{4\pi} \ln (\lambda/\bar{\lambda}) + \frac{\lambda}{\alpha\rho}\right\} \tag{14}$$

Extremization in ρ and λ gives $\lambda=\bar{\lambda}$ and $f = \bar{\lambda}/\alpha$.

The inverse square root of $\bar{\lambda}$ can be identified with the De Gennes persistence length (3). Physically, this is seen when calculating the fluctuations of the surface elements $x(\xi)$ from (11). At the extremum, they have a correlation function $(k^4+\bar{\lambda}k^2)^{-1}$, so that the length scale is indeed $(\bar{\lambda})^{-1/2}$.

We now go over to two membranes, following (11)-(14) and imposing a repulsion condition of the type (5). This gives the free energy

$$f = \rho \left\{ \frac{T}{2}\int\frac{d^2k}{(2\pi)^2}\left[\ln(G^{-1}(k)) - 2\ln(k^2(k^2+\lambda))\right] - T\frac{\lambda}{4\pi}\ln(\lambda/\bar{\lambda}) + \frac{2\lambda}{\alpha\rho} - \frac{\gamma}{4\alpha}\varepsilon d^2 \right\} \quad (15)$$

where $G^{-1}(k)=\binom{AB}{BA}$ with $A=k^6+\lambda k^2+\gamma/2$, $B=-\gamma/2$. Maximizing f in γ gives now

$$\frac{x^2}{4} = \frac{T}{2}\int\frac{d^2q}{(2\pi)^2}\frac{1}{A-B} = \frac{1}{4\pi}(4-\lambda_\gamma)\ \mathrm{atg}\left(\sqrt{4-\lambda_\gamma}/\lambda_\gamma\right) \quad (16a)$$

where

$$x^2 \equiv \sqrt{\gamma}\,\varepsilon\ d^2/\alpha \quad , \quad \lambda_\gamma \equiv \lambda/\sqrt{\gamma} \quad (16b)$$

The right-hand side is a function of the dimensionless ratio λ/λ_γ as shown in Fig. 1a. For λ=0, we recover the previous result (8) in the form x^2=1/4, for small λ_γ, $x^2 \approx (1/4)(1-\lambda_\gamma/\pi+...)$. For large λ_γ, $x^2 \approx (1/\pi\lambda_\gamma)\ln(\lambda_\gamma)$.

Minimizing f with respect to ρ gives $\lambda/\bar{\lambda}$ as a function of $\lambda \approx \gamma$

$$\ln(\lambda/\bar{\lambda}) = \frac{1}{2}\ln\lambda_\gamma + \frac{1}{2\lambda_\gamma}\sqrt{4-\lambda_\gamma}\ \mathrm{atg}\left(\sqrt{4-\lambda_\gamma}/\lambda_\gamma\right) - \pi x^2\lambda_\gamma$$

It is plotted in Fig. 1b. For small λ_γ, $\ln(\lambda/\bar{\lambda}) \approx (\pi/4\lambda_\gamma)(1-\lambda_\gamma/\pi + ...)$, for large λ_γ, $\ln(\lambda/\bar{\lambda}) \approx (1/\lambda_\gamma^2)\,[\ln(\lambda_\gamma)+1/2+...]$.

Maximizing f in λ, finally, implies that $f=\lambda/\alpha$. The result depends on two mass scales $M^2 \equiv \bar{\lambda}/\alpha$ and $1/d_0^2 \equiv (\bar{\lambda}\varepsilon/\alpha)$. The first is proportional to ζ^{-2}, i.e the transverse smoothless scale of the membranes and the overall size of f. The second is related to the interpenetrability of the two membranes and regulates how the energy depends on the distance d. In terms of m^2 we have $x^2=m^2d^2\lambda/\bar{\lambda}\lambda_\gamma$.

The energy $f=M^2\ \lambda/\bar{\lambda}$ is plotted in units M=1 as a function of $d\cdot m$. Its derivative $-(\partial/\partial d)f$ gives directly the pressure. For comparison, we display also the pure $1/d^2$ law of Helfrich's and see how the curve goes over from $\approx 1/d^2$ at short-distance to an exponential falloff at distance. For small d, $\lambda/\bar{\lambda}\approx 4/\pi d^2(1-4\ln\pi d^2)$. For large d, $\lambda/\bar{\lambda}\approx\exp\left[-2\pi(d/d_0)^2\right]$.

Notice that while the parameter $\bar{\lambda}$ can be calculated from the short distance cutoff Λ^{-1}, i.e. the molecular scale, and the membrane stiffness $1/\alpha$, via Eq. (13), the parameter d_0 is at present theoretically unaccessible. This is due to our incompetence of calculating path integrals with hard-wall constraints. Up to now, only computer simulations have been able to determine the related overall size c in the pressure law (a).[2)]

References

1) W. Helfrich, Z. Naturf. *A33*, 305(1978);

see also: W. Helfrich, R.M. Servuss, Nuovo Cimento *D3*, 137(1984);

,. Bivas, A.G. Petrov, J. Theor. Biol. *88*, 4598(1981);

D. Sornette, N. Ostrowski, J. Phys. (Paris) *45*(1984).

2) W. Janke, H. Kleinert, Phys. Lett. *A117*, 353(1986);

Phys. Rev Lett. *58*, 144(1987);

W.Janke, H. Kleinert, M. Meinhart, Berlin preprint 1988;

W, Janke, H. Kleinert, Berlin preprint 1988.

3) We use the same notation as in H. Kleinert, Phys. Rev. Lett. *58,* 1915(1987),

Phys. Lett. *B189*, 187(1987).

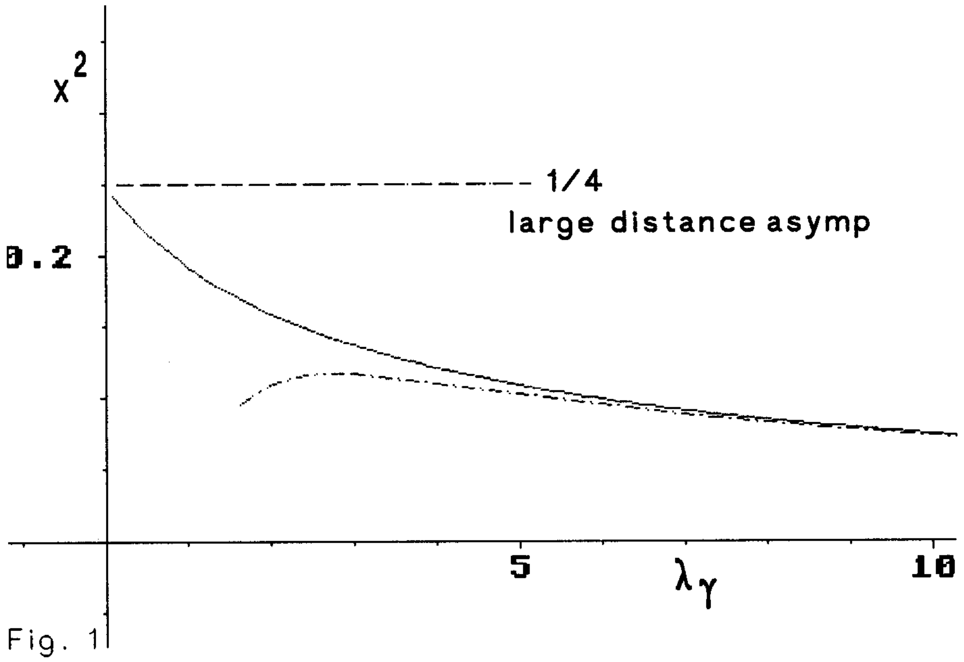

Fig. 1

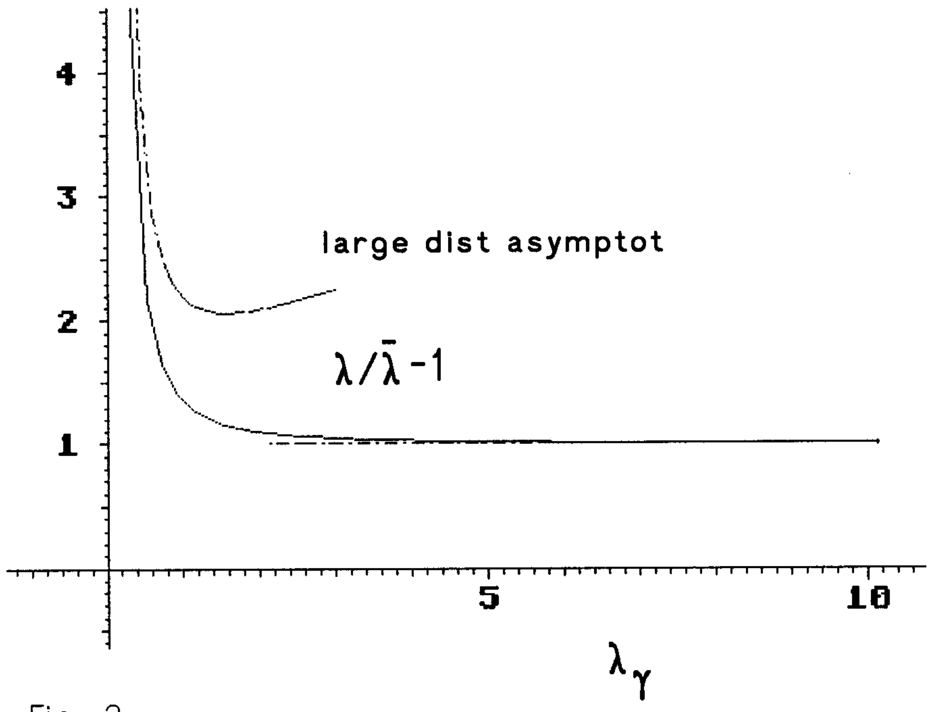

Fig. 2

Fig. 1a,b)

The solutions of the extremalizing conditions $\partial f/\partial\gamma=0$, $\partial f/\partial\rho=0$, showing $x^2=\gamma\varepsilon d^2/\alpha$ and $\lambda/\bar{\lambda}$.

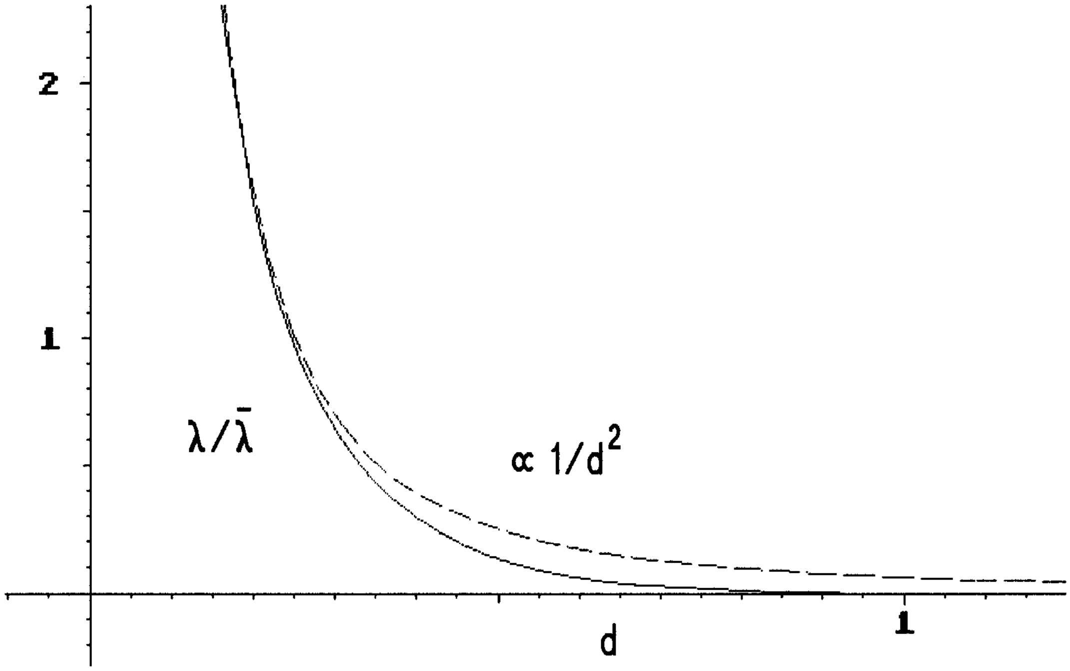

Fig. 3

Fig. 2)

The reduced free energy $f/M^2-1=\lambda/\bar{\lambda}-1$ as a function of the distance d/d_0 where M^{-1} and d_0 are the two length scales of the system (M^{-1} for the persistence of the stiffness and d_0 for the non-interpenetrability of the membranes).