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Fluctuation pressure of membrane between walls

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Abstract

For a single membrane of stiffness κ fluctuating between two planar walls of distance d, we calculate analytically the pressure law

$$p = \frac{\pi^2}{128}\frac{k_B^2 T^2}{\kappa (d/2)^3}.$$

The prefactor $\pi^2/128 \sim 0.077115\ldots$ is in very good agreement with results from Monte Carlo simulations 0.079 ± 0.002.

1. A stack of n parallel, thermally fluctuating membranes exerts upon the enclosing planar walls a pressure which depends on the stiffness κ and the temperature T as follows:

$$p = \alpha_n \frac{2n}{n+1}\frac{k_B^2 T^2}{\kappa [d/(n+1)]^3}, \tag{1}$$

where k_B is Boltzmann's constant and d the distance between the walls (see Fig. 1).

This law, first deduced from dimensional considerations by Helfrich [1], is of fundamental importance in the statistical mechanics of membranes just as the ideal gas law $pV = Nk_B T$ in the statistical mechanics of point particles. We would therefore like to know the size of the prefactor, the *stack constant* α_n as accurately as possible. So far, its value was determined only by extensive Monte Carlo simulations as being [2,3]

$$\alpha_\infty = 0.101 \pm 0.002. \tag{2}$$

For a single membrane, the following value was found [4,3]:

$$\alpha_1 = 0.079 \pm 0.002. \tag{3}$$

So far, there exists no analytic theory to explain these values.

The purpose of this note is to fill this gap for the constant α_1, by calculating analytically the pressure of a single membrane between parallel walls. The

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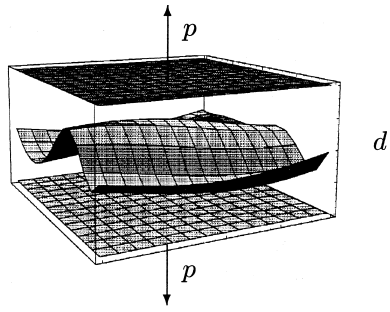

Fig. 1. Membrane fluctuating between walls of distance d, exerting a pressure p.

theoretical tool for this has only recently become available: A strong-coupling theory developed originally in quantum mechanics [5], was extended successfully to quantum field theories [6], where it has been used to obtain extremely accurate values for the critical exponents of O(n)-symmetric scalar fields with φ^4-interactions [6].

2. Strong-coupling theory gives direct access to the large-g behavior of divergent truncated power series expansions of the type

$$f_N(g) = \Omega\left[a_0 + \sum_{k=1}^{N} a_k \left(\frac{g}{\Omega^q}\right)^k\right]. \tag{4}$$

The $g\to\infty$-limit of $f_N(g)$, to be denoted by f_N^*, is obtained by setting $\Omega \equiv cg^{1/q}$ and optimizing the function

$$f_N(c) = g^{1/q}\tilde{f}_N(c) \equiv g^{1/q}\left(ca_0 b_0^N + \sum_{k=1}^{N} a_k c^{1-qk} b_k^N\right), \tag{5}$$

where

$$b_k^N = \sum_{l=0}^{N-k} (-1)^l \binom{(1-kq)/2}{l} \tag{6}$$

is the binomial expansion of $(1-1)^{(1-kq)/2}$ truncated after the $(N-k)$th term. Optimizing means extremizing $\tilde{f}_N(c)$ in c or, if an extremum does not exist, extremizing the derivative $\tilde{f}_N'(c)$.

3. We apply this theory to a membrane between walls by proceeding as follows. The partition function of the membrane is given by the functional integral

$$Z = \int \mathscr{D}u(x) \exp\left\{-\frac{\kappa}{2k_B T}\int d^2x \left[\partial^2 u(x)\right]^2\right\} \equiv e^{-Af/k_B T}, \tag{7}$$

where $u(x)$ is a vertical displacement field of the membrane fluctuating between horizontal walls at $u=-d/2$ and $d/2$. The quantities A and f are the wall area and the free energy per unit area, respectively. Such a restriction of a field is hard to treat analytically.

We therefore perform a transformation which maps the interval $u\in(-d/2,d/2)$ to an infinite φ-axis,

$$u = \frac{d}{\pi}\arctan\frac{\pi\varphi}{d} = \varphi\left(1 - \frac{\pi^2\varphi^2}{3d^2} + \frac{\pi^4\varphi^4}{5d^4} + \dots\right), \tag{8}$$

and add to the fluctuation energy E in the exponent of (7) a potential energy which keeps the membrane between $-d/2$ and $d/2$ (Pöschl–Teller potential):

$$E^{\rm pot} = E_0^{\rm pot} + E^{\rm int} = \frac{\kappa}{2}\int d^2x\, m^4\phi^2(u(x)) = \frac{\kappa m^4}{2}\int d^2x\left\{u^2(x) + \sum_{k=2}^{\infty}\varepsilon_k\left[\pi\frac{u(x)}{d}\right]^{2k}\right\}, \tag{9}$$

with expansion coefficients $\varepsilon_2,\varepsilon_3,\varepsilon_4,\dots$:

$$\tfrac{1}{3}, \tfrac{17}{90}, \tfrac{31}{315}, \tfrac{691}{14175}, \tfrac{10922}{467775}, \dots. \tag{10}$$

The potential energy per area is plotted in Fig. 2. Its presence destroys the simple scaling properties of the partition function (7), which depends only on the

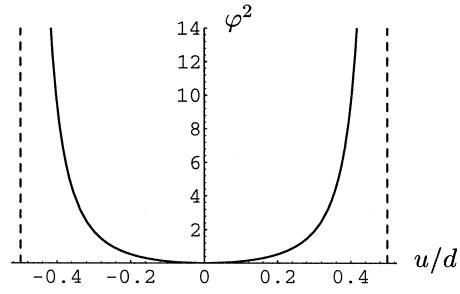

Fig. 2. Smooth Potential replacing box walls.

dimensionless variable $\kappa d^2/k_B T$. The new partition function Z associated with the modified energy $E + E^{\rm pot}$ has an additional dependence on the dimensionless variable $g = \pi^2/m^2 d^2$. The original hard-wall system is obtained in the strong-coupling limit $g \to \infty$.

In the opposite limit where g goes to zero, the energy $E + E^{\rm pot}$ becomes harmonic,

$$E_0 = \frac{\kappa}{2}\int d^2x \Big\{ \big[\partial^2 u(x)\big]^2 + m^4 u^2(x)\Big\}, \tag{11}$$

leading to a partition function

$$Z_0 = e^{-\frac{1}{2}{\rm Trlog}(\partial^4 + m^4)} = {\rm const} \times e^{-\frac{A}{8}m^2}, \tag{12}$$

where A is the area of the walls.

For a finite distance d, the interaction energy $E^{\rm int}$ is treated perturbatively order by order in g, expanding the exponential $e^{-E^{\rm int}/k_B T}$ in a power series, and each power in a sum of all pair contractions. These are pictured by loop diagrams whose lines represent the correlation function

$$\langle u(x_1) u(x_2)\rangle = \frac{\kappa}{k_B T}\int \frac{d^2k}{(2\pi)^2}\frac{1}{k^4 + m^4} e^{ik(x_1 - x_2)}. \tag{13}$$

The free energy density $f = -k_B T A^{-1} \log Z$ is obtained from all connected loop diagrams. For simplicity, we shall use natural units with $\kappa/k_B T = 1$.

The lowest contribution to the free energy density comes from the expectation value of the u^4-interaction or the loop diagram $3\bigcirc\!\!\!\!\bigcirc$ which is of the order $1/d^2$:

$$\frac{m^4}{2d^2}\langle u^4\rangle = \frac{m^4}{2d^2} 3\langle u^2\rangle^2, \tag{14}$$

the line representing the pair expectation

$$\langle u^2\rangle = \int \frac{d^2k}{(2\pi)^2}\frac{1}{k^4 + m^4} = \frac{1}{8m^2}. \tag{15}$$

Together with the exponent in (12), we thus obtain first-order free energy density

$$f_1 = \frac{m^2}{8} + \frac{1}{32}\frac{\pi^2}{m^2 d^2}. \tag{16}$$

Continuing the perturbation expansion, yields an expansion of the general form

$$f_N = m^2\left[\tfrac{1}{8} + \frac{1}{64}\frac{\pi^2}{m^2 d^2} + a_2\left(\frac{\pi^2}{m^2 d^2}\right)^2 + \ldots + a_N\left(\frac{\pi^2}{m^2 d^2}\right)^N\right], \tag{17}$$

where $a_2, \ldots, a_N$ are dimensionless numbers. By comparison with (4) we identify $p = q = 1$, $\Omega = m^2$, $g = \pi^2/d^2$. The function $f_N(c)$ of Eq. (5) describing the limiting large-g behavior is obtained by setting $\Omega \equiv c\pi^2/2d^2$, and reads

$$f_N(c) = \frac{\pi^2}{d^2}\left(\frac{c}{4} b_0^N + \tfrac{1}{64} + \frac{a_2}{c} b_2^N + \ldots + \frac{a_N}{c^{N-1}} b_N^N\right). \tag{18}$$

According to the above-described strong-coupling theory, we must optimize the expression $\tilde{f}_N(c)$ in parentheses. Since the second term does not contain c, we separate this term out, and write

$$\tilde{f}_N(c) = \tfrac{1}{64} + \Delta\tilde{f}_N(c) \equiv \tfrac{1}{64} + \left(\frac{c}{4} b_0^N + \frac{a_2}{c} b_2^N + \ldots + \frac{a_N}{c^{N-1}} b_N^N\right), \tag{19}$$

with only the remainder $\Delta\tilde{f}_N(c)$ to be optimized. Let $\Delta\tilde{f}_N^*$ be ist optimal value. If we know only a_2, we find the approximation $\Delta f_2^* = \sqrt{3a_2/16}$. Ignoring Δf_N^* for a moment, the first term in (19) yields the lowest estimate for the free energy density of the original system

$$f_1^* = \frac{\pi^2}{64}\frac{1}{d^2}, \tag{20}$$

implying a pressure law

$$p = -\frac{\partial f}{\partial d} = \frac{\pi^2}{32}\frac{1}{d^3}. \tag{21}$$

By comparison with the general pressure law (1), we identify the prefactor as being

$$\alpha_1 = \tfrac{1}{2} \times \frac{\pi^2}{128} \approx \tfrac{1}{2} \times 0.077115. \tag{22}$$

Without the prefactor factor $1/2$, this would agree perfectly with the Monte Carlo value (3). Thus we expect the contribution of $\Delta\tilde{f}_N^*$ for $N\to\infty$ to be equal or almost equal to $1/64$.

The calculation of the higher-order terms $a_2, a_3, \dots$ is tedious, and will be presented in a separate detailed publication [7]. In this note we shall circumvent it by exploiting a close relationship of the present problem with a closely analogous exactly solvable one, which may be treated in precisely the same way: The euclidean version of a quantum-mechanical point particle in a one-dimensional box $u\in(-d/2,d/2)$.

4. The partition function of a particle in a box is

$$Z=\int\mathscr{D}u\,\mathrm{e}^{-(\kappa/2k_{\mathrm{B}}T)\int dx(\partial u)^2}\equiv\mathrm{e}^{-Af/k_{\mathrm{B}}T}. \tag{23}$$

The quantum-mechanical ground state energy of this system is exactly known: $(k_{\mathrm{B}}T/\kappa)\pi^2/2d^2$, corresponding to a free energy density

$$f=\frac{k_{\mathrm{B}}^2T^2}{\kappa}\,\frac{\pi^2}{2d^2}. \tag{24}$$

The path integral (23) may now be treated as before, i.e., we transform u to φ via (8), and separate the field energy into a Gaussian energy (in natural units)

$$E_0=\frac{\kappa}{2}\int dx\Big\{\big[\partial^2u(x)\big]^2+m^4u^2(x)\Big\} \tag{25}$$

and an interaction energy which looks the same as (9), except that the integration $\int d^2x$ runs now only over one dimension, $\int dx$.

The first-order contribution to the free energy density is now (in natural units with $\kappa/k_{\mathrm{B}}T=1$)

$$\frac{m^4}{2d^2}\langle u^4\rangle=\frac{m^4}{2d^2}3\langle u^2\rangle^2, \tag{26}$$

with the pair expectation

$$\langle u^2\rangle=\int\frac{dq}{2\pi}\,\frac{1}{q^2+m^4}=\frac{1}{2m^2}, \tag{27}$$

leading to a first-order free energy density

$$f_1=\frac{m^2}{2}+\frac{1}{2}\,\frac{\pi^2}{d^2}, \tag{28}$$

and a full perturbation expansion of the form

$$f=m^2\left(\tfrac{1}{2}+\frac{1}{2}\,\frac{\pi^2}{m^2d^2}+a_2\frac{\pi^4}{m^4d^4}+\dots\right). \tag{29}$$

From this we find the function $f_N(c)$ defined in Eq. (5) governing the strong-coupling limit $d\to0$ by setting $\Omega=m^2\equiv c\pi^2/2d^2$:

$$f_N(c)=\frac{\pi^2}{d^2}\,\tilde{f}_N(c), \tag{30}$$

with

$$\tilde{f}_N(c)=\tfrac{1}{4}+\Delta\tilde{f}_N(c)\equiv\tfrac{1}{4}+\left(\frac{c}{4}b_0^N+\frac{a_2}{c}b_2^N+\dots+\frac{a_N}{c^{N-1}}b_N^N\right). \tag{31}$$

Here the first term yields the lowest approximation

$$f_1=\frac{1}{4}\,\frac{\pi^2}{d^2}, \tag{32}$$

which is *precisely* half the exact result. Thus we conclude that the optimal value of the neglected expression $\Delta f_N(c)$ must be once more equal to $1/4$ in the limit $N\to\infty$. In order to see how this happens, we extend the Bender–Wu recursion relation for the perturbation coefficients of the anharmonic oscillator [8]. It yields for the ground state energy an expansion

$$\begin{aligned}&\tfrac{1}{2}+\frac{3\pi^2}{4d^2}\varepsilon_4-\frac{\pi^4}{8d^4}\big(21\varepsilon_4^2-15\varepsilon_6\big)\\&+\frac{\pi^6}{16d^6}\big(333\varepsilon_4^3-360\varepsilon_4\varepsilon_6+105\varepsilon_8\big)\\&-\frac{\pi^8}{128d^8}\big(30885\varepsilon_4^4-44880\varepsilon_4^2\varepsilon_6+6990\varepsilon_6^2\\&+1512\varepsilon_4\varepsilon_8+3780\varepsilon_{10}\big)+\dots.\end{aligned} \tag{33}$$

Inserting the coefficients (10) we find $a_2,a_4,a_6,\dots$:

$$\tfrac{1}{16},-\tfrac{1}{256},\tfrac{1}{2048},-\tfrac{5}{65536},\tfrac{7}{524288},-\tfrac{21}{8388608},\dots, \tag{34}$$

whereas the odd coefficients $a_3,a_5,a_7,\dots$ vanish.

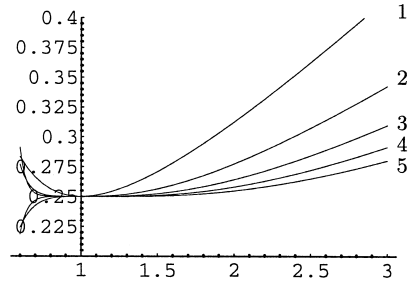

Fig. 3. Plots of the functions $\Delta\tilde{f}_N(c)$ of Eq. (35), all being optimal exactly at $c=1$ with $\Delta\tilde{f}_N^*=1/4$.

Table 1
The functions $\Delta\tilde{f}_N(c)$ of Eq. (35), and their optimal values $\Delta\tilde{f}_N^*$

N	$\Delta\tilde{f}_N(c)$	$\Delta\tilde{f}_N^*$
1	$\frac{c}{4}+\frac{c^{-1}}{16c}$	$\frac{1}{4}$
2	$\frac{3c}{16}+\frac{3c^{-1}}{32}-\frac{c^{-3}}{256}$	$\frac{1}{4}$
3	$\frac{5c}{32}+\frac{15c^{-1}}{128}-\frac{5c^{3}}{512}+\frac{c^{-5}}{2048}$	$\frac{1}{4}$
4	$\frac{35c}{256}+\frac{35c^{-1}}{256}-\frac{35c^{3}}{3048}+\frac{7c^{-5}}{4096}-\frac{5}{65536}$	$\frac{1}{4}$
5	$\frac{63}{512}+\frac{315c^{-1}}{2048}-\frac{105c^{3}}{4096}+\frac{63c^{-5}}{16384}-\frac{45c^{-7}}{131072}+\frac{7c^{-9}}{524288}$	$\frac{1}{4}$

To account for this fact, we resum the series containing only the even terms

$$\Delta\tilde{f}_N=\frac{c}{4}+\frac{a_2}{c}b_1^N+\frac{a_4}{c^3}b_2^N+\frac{a_{2N}}{c^5}b_N^N, \tag{35}$$

taking the coefficients b_i^N of Eq. (6) with the parameters $p=1, q=2$. This yields the functions $\Delta\tilde{f}_N(c)$ plotted in Fig. 3 and listed in Table 1. For all $\Delta\tilde{f}_N(c)$, optimization yields a strong-coupling value $\Delta\tilde{f}_N^*$ equal to $1/4$, thus raising the initial value $1/4$ in (31) to the correct final value $1/2$.

5. To exploit this property of a particle in a box for the system at hand, the membrane between walls, we make the following crucial observation: The Feynman integrals determining the first two terms in the free energy densities in Eq. (16) for a membrane and in Eq. (28) for a particle are related to each other by a simple transformation of the integration variables. The membrane integrals

$$\int\frac{d^2k}{(2\pi)^2}\log(k^4+m^4)=\frac{m^2}{4},$$
$$\int\frac{d^2k}{(2\pi)^2}\frac{1}{k^4+m^4}=\frac{1}{8m^2} \tag{36}$$

go over into those of the particle in the box

$$\int\frac{dq}{2\pi}\log(q^2+m^4)=m^2,\quad \int\frac{dq}{2\pi}\frac{1}{q^2+m^4}=\frac{1}{2m^2} \tag{37}$$

by the transformation

$$k^2\to q,\quad \int\frac{d^2k}{(2\pi)^2}\to\tfrac{1}{4}\int_{-\infty}^{\infty}\frac{dq}{2\pi}.$$

Thus, if we multiply each loop integral by a factor $1/4$, we find immediately the free energy density f_1 of the membrane in Eq. (16) from that of the particle in the box in Eq. (28).

But the analogy carries further: By differentiation (36) and (37) with respect to m^2, we see that also all Feynman integrals $\int d^2k/(2\pi)^2(k^4+m^4)^\nu$ are related to the $\int dq/(2\pi)(q^2+m^4)^\nu$ by the same factor $1/4$. This property has the consequence that *most* of the connected loop diagrams contributing to the perturbation expansion of the free energy density, shown in Fig. 4 up to five loops, are related by a factor $(1/4)^L$, where L is the number of loops. In particular, all such diagrams coincide which are usually summed in the Hartree–Fock approximation (chain diagrams, daisy diagrams, etc.). Only the topological more involved diagrams 3–1, 4–1, 4–2, 4–5, 5–2, 5–3, 5–5, 5–6, 5–7, 5–11, 5–12, 5–15 in Fig. 4 do not follow this pattern. For a particle in a box, we can easily calculate the associated Feynman integrals in x-space as described in Chapter 3 of Ref. [5], and find that they contribute less than 5% to the sum of all diagrams at each loop level. This implies that the corresponding results for the membrane between walls will differ at most by this relative amount from those for the particle in the box. We therefore conclude that since the optimal value of $\Delta\tilde{f}_N(c)$ in Eq. (31) doubles the initial value for $N\to\infty$, the analogous function for the membrane between walls in Eq. (19) will double approximately. For the quantitative deviations see the forthcoming publication [7]. A precise doubling of the result (22) leads to a very good agreement with the Monte Carlo number (2).

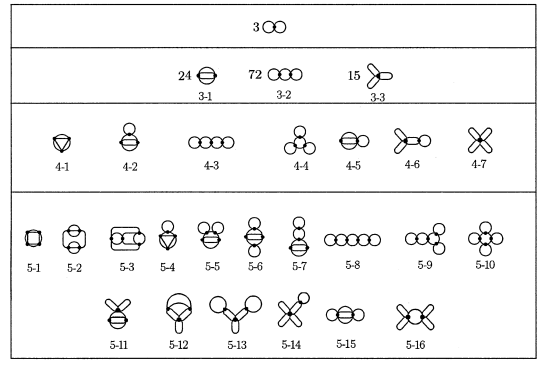

Fig. 4. Vacuum diagrams up to five loops.

6. The alert reader will have noted that the field transformation (8) is rather special. We may, for instance, chose any mapping

$$u = \frac{\varphi}{\left[1+8\pi^2\varphi^2/3d^2 + w_4\varphi^4/d^4 + \ldots + (2\varphi/d)^n\right]^{1/n}}$$

$$= \varphi - \tfrac{2}{3}\frac{\pi^2}{d^2}\varphi^3 + \ldots + \mathcal{O}(\varphi^5), \qquad (38)$$

which has a doubled coefficient of φ^3 with respect to the expansion (8). As a consequence, the functions $\tilde{f}_N(c)$ in (19) and (31) would have a doubled first term. Since this would be the correct final value, the remaining functions $\Delta\tilde{f}_N(c)$ would have to converge to a vanishing optimal value for $N\to\infty$ (in the particle case exactly, in the membrane case approximately). To reach this goal, the coefficients $w_4, w_6, \ldots$ in (38) can be chosen rather arbitrarily, although there are a few convenient ways for which the speed of convergence is fast. A preferred choice is one in which all coefficients $a_2, a_3, a_3, \ldots$ of the perturbation expansion vanishes for a particle in a box. This and other possibilities will be studied separately [9,10].

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