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# Strong-coupling calculation of fluctuation pressure of a membrane between walls

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## Abstract

We calculate analytically the proportionality constant in the pressure law of a membrane between parallel walls from the strong-coupling limit of variational perturbation theory up to third order. Extrapolating the zeroth to third approximations to infinity yields the pressure constant  $\alpha = 0.0797149$ . This result lies well within the error bounds of the most accurate available Monte Carlo result  $\alpha^{\text{MC}} = 0.0798 \pm 0.0003$ . © 1999 Elsevier Science B.V. All rights reserved.

## 1. Membrane between walls

The violent thermal out-of-plane fluctuations of a membrane between parallel walls generate a pressure  $p$  following the law

$$p = \alpha \frac{k_B^2 T^2}{\kappa (d/2)^3}, \quad (1.1)$$

whose form was first derived by Helfrich [1]. Here,  $\kappa$  denotes the elasticity constant of the membrane, and  $d$  the distance between the walls. The exact value of the prefactor  $\alpha$  is unknown, but estimates have been derived from crude theoretical approxima-

tions by Helfrich [1] and by Janke and Kleinert [2] which yielded

$$\alpha_H^{\text{th}} \approx 0.0242, \quad \alpha_{\text{JK}}^{\text{th}} \approx 0.0625. \quad (1.2)$$

More precise values were found from Monte Carlo simulations by Janke and Kleinert [2] and by Gompper and Kroll [3] which gave

$$\alpha_{\text{JK}}^{\text{MC}} \approx 0.079 \pm 0.002, \quad \alpha_{\text{GK}}^{\text{MC}} \approx 0.0798 \pm 0.0003. \quad (1.3)$$

In previous work [4], a systematic method was developed for calculating  $\alpha$  with any desired high accuracy. Basis for this method is the strong-coupling version of variational perturbation theory [5]. In that theory, the free energy of the membrane is expanded into a sum of connected loop diagrams, which is eventually taken to infinite coupling strength to account for the hard walls. As a first approximation, an infinite set of diagrams was calculated, others were estimated by invoking a mathematical analogy with a

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similar one-dimensional system of a quantum mechanical particle between walls. The result of this procedure was a pressure constant

$$\alpha_K^{\text{th}} = \frac{\pi^2}{128} = 0.0771063\dots, \quad (1.4)$$

very close to (1.3).

It is the purpose of this Letter to go beyond this estimate by calculating all diagrams up to four loops exactly. In this way, we improve the analytic approximation (1.4) and obtain a value

$$\alpha^{\text{th}} \approx 0.0797149, \quad (1.5)$$

which is in excellent agreement with the precise MC value  $\alpha_{\text{GK}}^{\text{MC}}$  in Eq. (1.3).

## 2. The smooth potential model of the membrane between walls

To set up the theory, we let the membrane lie in the  $\mathbf{x}$ -plane and fluctuate in the  $z$ -direction with vertical displacements  $\varphi(\mathbf{x})$ . The walls at  $z = \pm d/2$  restrict the displacements to the interval  $\varphi \in (-d/2, d/2)$ . Near zero temperature, the thermal fluctuations are small,  $\varphi(\mathbf{x}) \approx 0$ . The curvature energy  $E$  of the membrane has the harmonic approximation [1]

$$E = \frac{1}{2}\kappa \int d^2x \left[ \partial^2 \varphi(\mathbf{x}) \right]^2. \quad (2.1)$$

The thermodynamic partition function  $Z$  of the membrane is given by the sum over all Boltzmann factors of field configurations  $\varphi(\mathbf{x})$

$$Z = \prod_{\mathbf{x}} \left[ \int_{-d/2}^{+d/2} \frac{d\varphi(\mathbf{x})}{\sqrt{2\pi k_B T / \kappa}} \right] \times \exp \left\{ -\frac{\kappa}{2k_B T} \int d^2x \left[ \partial^2 \varphi(\mathbf{x}) \right]^2 \right\}. \quad (2.2)$$

This simple harmonic functional integral poses the problem of dealing with a finite range of fluctua-

tions. This problem is solved by the strong-coupling theory of Ref. [4] as follows.

If the area of the membrane is denoted by  $A$ , the partition function (2.6) determines the free energy per area as

$$f = -\frac{1}{A} \ln Z. \quad (2.3)$$

By differentiating  $f$  with respect to the distance  $d$  of the walls, we obtain the pressure  $p = -\partial f / \partial d$ .

### 2.1. Smooth potential adapting walls

We introduce some smooth potential restricting the fluctuations  $\varphi(\mathbf{x})$  to the interval  $(-d/2, d/2)$ , for instance

$$V(\varphi(\mathbf{x})) = m^4 \frac{d^2}{\pi^2} \tan^2 \frac{\pi}{d} \varphi(\mathbf{x}) \equiv m^4 \varphi^2(\mathbf{x}) + \frac{\pi^2}{d^2} V_{\text{int}}(\varphi(\mathbf{x})), \quad (2.4)$$

where we have split the potential into harmonic and interacting part

$$V_{\text{int}}(\varphi(\mathbf{x})) = m^4 \left[ \varepsilon_4 \varphi^4(\mathbf{x}) + \varepsilon_6 \left( \frac{\pi}{d} \right)^2 \varphi^6(\mathbf{x}) + \varepsilon_8 \left( \frac{\pi}{d} \right)^4 \varphi^8(\mathbf{x}) + \dots \right], \quad (2.5)$$

with  $\varepsilon_4 = 2/3, \varepsilon_6 = 17/45, \varepsilon_8 = 62/315, \dots$ . Thus we are left with the functional integral

$$Z = \oint \mathcal{D}\varphi(\mathbf{x}) \exp \left\{ -\frac{1}{2} \int d^2x \left\{ \left[ \partial^2 \varphi(\mathbf{x}) \right]^2 + m^4 \varphi^2(\mathbf{x}) + \frac{\pi^2}{d^2} V_{\text{int}}(\varphi(\mathbf{x})) \right\} \right\}, \quad (2.6)$$

where we have set  $\kappa = k_B T = 1$ . After truncating the Taylor expansion around the origin, the periodicity of the trigonometric function is lost and the integrals over  $\varphi(\mathbf{x})$  in (2.2) can be taken from  $-\infty$  to  $+\infty$ . The interacting part is treated perturbatively. Then, the harmonic part of  $V(\varphi(\mathbf{x}))$  leads to an exactly

integrable partition function  $Z_{m^2}$ . The mass parameter  $m$  is arbitrary at the moment, but will eventually be taken to zero, in which case the potential  $V(\varphi(\mathbf{x}))$  describes two hard walls at  $\varphi = \pm d/2$ .

We shall now calculate a perturbation expansion for  $Z$  up to four loops. This will serve as a basis for the limit  $m \rightarrow 0$ , which will require the strong-coupling theory of Ref. [4].

### 2.2. Perturbation expansion for free energy

The perturbation expansion proceeds from the harmonic part of Eq. (2.20):

$$Z_{m^2} = \oint \mathcal{D}\varphi(\mathbf{x}) e^{-\mathcal{A}_{m^2}[\varphi]/2} = e^{-A f_{m^2}}, \quad (2.7)$$

with

$$\mathcal{A}_{m^2}[\varphi] = \int d^2x \left\{ [\partial^2\varphi(\mathbf{x})]^2 + m^4\varphi^2(\mathbf{x}) \right\}. \quad (2.8)$$

From Refs. [2,4], the harmonic free energy per unit area  $f_{m^2}$  is known as

$$f_{m^2} = \frac{1}{8}m^2. \quad (2.9)$$

The harmonic correlation functions associated with (2.7) are

$$\begin{aligned} & \langle O_1(\varphi(\mathbf{x}_1)) O_2(\varphi(\mathbf{x}_2)) \cdots \rangle_{m^2} \\ &= \frac{1}{Z_{m^2}} \oint \mathcal{D}\varphi(\mathbf{x}) O_1(\varphi(\mathbf{x}_1)) \\ & \quad \times O_2(\varphi(\mathbf{x}_2)) \cdots e^{-\mathcal{A}_{m^2}[\varphi]/2}, \end{aligned} \quad (2.10)$$

where the functions  $O_i(\varphi(\mathbf{x}_j))$  may be arbitrary polynomials of  $\varphi(\mathbf{x}_j)$ . The basic harmonic correlation function

$$G_{m^2}(\mathbf{x}_1, \mathbf{x}_2) = \langle \varphi(\mathbf{x}_1) \varphi(\mathbf{x}_2) \rangle_{m^2} \quad (2.11)$$

determines, by Wick's rule, all correlation functions (2.10) as sums of products of (2.11):

$$\begin{aligned} & \langle \varphi(\mathbf{x}_1) \cdots \varphi(\mathbf{x}_n) \rangle_{m^2} \\ &= \sum_{\text{pairs}} G_{m^2}(\mathbf{x}_{P(1)}, \mathbf{x}_{P(2)}) \cdots G_{m^2}(\mathbf{x}_{P(n-1)}, \mathbf{x}_{P(n)}), \end{aligned} \quad (2.12)$$

where the sum runs over all pair contractions, and  $P$  denotes the associated index permutations. The harmonic correlation function (2.11) is in momentum space

$$G_{m^2}(\mathbf{k}) = \frac{1}{k^4 + m^4} = \frac{i}{2m^2} \left[ \frac{1}{k^2 + im^2} - \frac{1}{k^2 - im^2} \right], \quad (2.13)$$

thus being proportional to the difference of two ordinary correlation functions  $(p^2 - \mu^2)^{-1}$  with an imaginary square mass  $\mu^2 = \pm im^2$ . From their known  $\mathbf{x}$ -space form we have immediately

$$\begin{aligned} G_{m^2}(\mathbf{x}_1, \mathbf{x}_2) &= G_{m^2}(\mathbf{x}_1 - \mathbf{x}_2) \\ &= \frac{i}{4\pi m^2} \left[ K_0(\sqrt{i}m|\mathbf{x}_1 - \mathbf{x}_2|) \right. \\ & \quad \left. - K_0(\sqrt{-i}m|\mathbf{x}_1 - \mathbf{x}_2|) \right], \end{aligned} \quad (2.14)$$

where  $K_0(z)$  is a modified Bessel function [6]. At zero distance, the ordinary harmonic correlations are logarithmically divergent, but the difference is finite yielding  $G_{m^2}(0) = 1/8m^2$ .

We now expand the partition function (2.6) in powers of  $gV_{\text{int}}(\varphi(\mathbf{x}))$ , where  $g \equiv \pi^2/d^2$ , and use (2.10) to obtain a perturbation series for  $Z$ . Going over to the cumulants, we find the free energy per unit area

$$\begin{aligned} f &= f_{m^2} + \frac{g}{2A} \int d^2x \langle V_{\text{int}}(\varphi(\mathbf{x})) \rangle_{m^2, c} \\ & \quad - \frac{g^2}{2!} \frac{1}{4A} \int d^2x_1 d^2x_2 \langle V_{\text{int}}(\varphi(\mathbf{x}_1)) \\ & \quad \times V_{\text{int}}(\varphi(\mathbf{x}_2)) \rangle_{m^2, c} + \dots, \end{aligned} \quad (2.15)$$

where the subscript  $c$  indicates the cumulants. Inserting the expansion (2.5) and using (2.10) and (2.12), the series can be written as

$$f = m^2 \left[ a_0 + \sum_{n=1}^{\infty} a_n \left( \frac{g}{m^2} \right)^n \right], \quad (2.16)$$

where the coefficients  $a_n$  are dimensionless real numbers, starting with  $a_0 = 1/8$ . The higher expansion

sion coefficients  $a_n$  are combinations of integrals over the connected correlation functions:

$$a_1 = \varepsilon_4 \frac{m^2}{2A} \int d^2x \langle \varphi^4(\mathbf{x}) \rangle_{m^2, c}, \quad (2.17)$$

$$a_2 = \varepsilon_6 \frac{m^6}{2A} \int d^2x \langle \varphi^6(\mathbf{x}) \rangle_{m^2, c} \\ - \varepsilon_4^2 \frac{m^{10}}{8A} \int d^2x_1 d^2x_2 \langle \varphi^4(\mathbf{x}_1) \varphi^4(\mathbf{x}_2) \rangle_{m^2, c}, \quad (2.18)$$

$$a_3 = \varepsilon_8 \frac{m^8}{2A} \int d^2x \langle v^8(\mathbf{x}) \rangle_{m^2, c} \\ - \varepsilon_4 \varepsilon_6 \frac{m^{12}}{4A} \int d^2x_1 d^2x_2 \langle \varphi^6(\mathbf{x}_1) \varphi^4(\mathbf{x}_2) \rangle_{m^2, c} \\ + \varepsilon_4^3 \frac{m^{16}}{48A} \int d^2x_1 d^2x_2 d^2x_3 \langle \varphi^4(\mathbf{x}_1) \\ \times \varphi^4(\mathbf{x}_2) \varphi^4(\mathbf{x}_3) \rangle_{m^2, c}. \quad (2.19)$$

To find the free energy (2.16) between walls, we must go to the limit  $m^2 \rightarrow 0$ . Following [4,5], we substitute  $m^2$  by the variational parameter  $M^2$ , which is introduced via the trivial identity  $m^2 \equiv \sqrt{M^4 - gr}$  with  $r = (M^4 - m^4)/g$ , and expand this in powers of  $g$  up to the order  $g^N$ . In the limit  $m^2 \rightarrow 0$ , this expansion reads

$$m^2(M^2) = M^2 - \frac{1}{2} \frac{r}{M^2} g - \frac{1}{8} \frac{r^2}{M^6} g^2 \\ - \frac{1}{16} \frac{r^3}{M^{10}} g^3 - \dots \quad (2.20)$$

Inserting this into (2.16), reexpanding in powers of  $g$ , and truncating after the  $N$ th term, we arrive at the free energy per unit area

$$f_N(M^2, d) = M^2 a_0 b_0 + \sum_{n=1}^N a_n g^n M^{2(1-n)} b_n, \quad (2.21)$$

with

$$b_n = \sum_{k=0}^{N-n} (-1)^k \binom{(1-n)/2}{k} \quad (2.22)$$

being the binomial expansion of  $(1-1)^{(1-n)/2}$  truncated after the  $(N-n)$ th term [4]. The optimization

of (2.21) is done as usual [5] by determining the minimum of  $f_N(M^2, d)$  with respect to the variational parameter  $M^2$ , i.e. by the condition

$$\frac{\partial f_N(M^2, d)}{\partial M^2} \stackrel{!}{=} 0, \quad (2.23)$$

whose solution gives the optimal value  $M_N^2(d)$ . Re-substituting this result into Eq. (2.21) produces the optimized free energy  $f_N(d) = f_N(M_N^2(d), d)$ , which only depends on the distance as  $f_N(d) = 4\alpha_N/d^2$ . Its derivative with respect to  $d$  yields the desired pressure law with the  $N$ th order approximation for the constant  $\alpha_N$ :

$$p_N = \alpha_N \left( \frac{d}{2} \right)^{-3}. \quad (2.24)$$

We must now calculate the cumulants occurring in the expansion (2.16).

### 3. Evaluation of the fluctuation pressure up to four-loop order

The correlation functions appearing in (2.17)–(2.19) are conveniently represented by Feynman graphs. Green functions are pictured as solid lines and local interactions as dots, whose coordinates are integrated over:

$$\mathbf{x}_1 \text{---} \mathbf{x}_2 \equiv G_{m^2}(\mathbf{x}_1, \mathbf{x}_2), \quad (3.1)$$

$$\bullet \equiv \int d^2x. \quad (3.2)$$

These rules can be taken over to momentum space in the usual way. One easily verifies that the integrals over the connected correlation functions in (2.17)–(2.19) have a dimension  $A/m^{2(n+V-1)}$ , where  $V$  is the number of the vertices of the associated Feynman diagrams. Thus we parametrize each Feynman diagram by  $vA/m^{2(n+V-1)}$ , with a dimensionless number  $v$ , which includes the multiplicity. In Table 1, we have listed the values  $v$  for all diagrams up to four loops. No divergences are encountered. Exact results are stated as fractional numbers. The other numbers are obtained by numerical integration, which are reliable up to the last written digit. The right-hand column shows numbers  $v_K$  obtained by the earlier approximation [4], where all the Feynman diagrams

Table 1  
Feynman diagrams with loops  $L$ , multiplicities  $s$ , and their dimensionless values  $v$ . The last column shows the values  $v_K = v_{PB}/4^L$  used in Ref. [4].

$L$	Graph	$s$	$v$	$v_K$
2		3	$\frac{3}{64}$	$\frac{3}{64}$
			$a_1 = a_1^K$	$a_1^K = 1/64$
3		15	$\frac{15}{512}$	$\frac{15}{512}$
		72	$\frac{9}{128}$	$\frac{9}{128}$
		24	$0.828571 \times \frac{3}{256}$	$\frac{3}{256}$
		$a_2 = 1.114286 a_2^K$		$a_2^K = 1/1024$
4		105	$\frac{105}{4096}$	$\frac{105}{4096}$
		540	$\frac{135}{2048}$	$\frac{135}{2048}$
		360	$0.828571 \times \frac{45}{2048}$	$\frac{45}{2048}$
		2592	$\frac{81}{512}$	$\frac{81}{512}$
		1728	$\frac{81}{512}$	$\frac{81}{512}$
		3456	$0.828571 \times \frac{135}{1024}$	$\frac{135}{1024}$
		1728	$0.713194 \times \frac{81}{2048}$	$\frac{81}{2048}$
		$a_3 = 2.763097 \cdot 10^{-5}$		$a_3^K = 0$

were estimated by an analogy to the the problem of a particle in a box. In Ref. [4], it was shown that the value  $v$  of a large class of diagrams of the membrane problem can be obtained by simply dividing the value of the corresponding particle-in-a-box-diagram  $v_{PB}$  by a factor  $1/4^L$ , where  $L$  is the number of loops in the diagrams.

Inserting the numbers in Table 1 into (2.17)–(2.19), we obtain the coefficients  $a_1, a_2, a_3$  of the free energy per area (2.21), which is then extremized

in  $M^2$ . To see how the results evolve from order to order, we start with the first order

$$f_1(M^2, d) = \frac{1}{2} a_0 M^2 + a_1 \frac{\pi^2}{d^2}, \tag{3.3}$$

with  $a_0 = 1/8$  and  $a_1 = 1/64$ . Here, an optimal value of  $M^2$  does not exist. Thus we simply use the perturbative result for  $m = 0$  which is equal to (3.3) for  $M = 0$ . Differentiating  $f_1(0, d)$  with respect to  $d$  yields the pressure constant in (2.24):

$$\alpha_1 = \frac{1}{4} a_1 \frac{\pi^2}{d^2} = \frac{\pi^2}{256} \approx 0.038553. \tag{3.4}$$

This value is about half as big as the Monte Carlo estimates (1.3) and agrees with the value found in [4]. To second order, the reexpansion (2.21) reads

$$f_2(M^2, d) = \frac{3}{8} a_0 M^2 + a_1 \frac{\pi^2}{d^2} + a_2 \frac{\pi^4}{d^4} \frac{1}{M^2} \tag{3.5}$$

with  $a_2 \approx 1.0882 \cdot 10^{-3}$  from Table 1. Minimizing this energy in  $M^2$  yields an optimal value

$$M_2^2(d) = \sqrt{\frac{8}{3} \frac{a_2}{a_0}} \frac{\pi^2}{d^2} \approx 0.152362 \frac{\pi^2}{d^2}, \tag{3.6}$$

and

$$f_2(d) = \frac{\pi^2}{d^2} \left( a_1 + \sqrt{\frac{3}{2} a_0 a_2} \right). \tag{3.7}$$

Inserting  $a_0 = 1/8$  and  $a_1, a_2$  from Table 1, we obtain

$$\alpha_2 \approx 0.073797, \tag{3.8}$$

thus improving drastically the first-order estimate (3.4) This value is by a factor 1.026 larger than that obtained in the approximation of Ref. [4].

Continuing this proceeding to third order, we must minimize

$$f_3(M^2, d) = \frac{5}{16} a_0 M^2 + a_1 \frac{\pi^2}{d^2} + \frac{3}{2} a_2 \frac{\pi^4}{d^4} \frac{1}{M^2} + a_3 \frac{\pi^6}{d^6} \frac{1}{M^4}, \tag{3.9}$$

with  $a_3 \approx 2.7631 \cdot 10^{-5}$ . The optimal value of  $M^2$  is

$$M_3^2(d) = \sqrt{\frac{32}{5} \frac{a_2}{a_0}} \cos \left[ \frac{1}{3} \arccos \sqrt{\frac{5}{2} \frac{a_0 a_3^2}{a_2^3}} \right] \frac{\pi^2}{d^2} \approx 0.219608 \frac{\pi^2}{d^2}. \quad (3.10)$$

Inserted into (3.9), we find the four-loop approximation for the proportionality constant  $\alpha$ :

$$\alpha_3 \approx 0.079472. \quad (3.11)$$

This result is in very good agreement of the Monte Carlo results in (1.3). It differs from the approximate value of the method presented in Ref. [4] by a factor 1.047.

An even better result will now be obtained by extrapolating the sequence  $\alpha_1, \alpha_2, \alpha_3$  to infinite order.

#### 4. Extrapolation towards the exact constant

Variational perturbation theory exhibits typically an exponentially fast convergence. This was exactly proven for the anharmonic oscillator [5]. Other systems treated by variational perturbation theory show a similar behavior [7]. Assuming that an exponential convergence exists also here, we may extrapolate the sequence of values  $\alpha_1, \alpha_2, \alpha_3$  calculated above to infinite order. It is useful to extend this sequence by one more value at the lower end,  $\alpha_0 = 0$ , which follows from the one-loop energy (2.9) at  $m^2 = 0$ . This sequence is now extrapolated towards a hypothetical exact value  $\alpha_{\text{ex}}$  by parametrizing the approach as

$$\alpha_{\text{ex}} - \alpha_N = \exp(-\eta - \xi N^\epsilon). \quad (4.1)$$

The parameters  $\eta$ ,  $\xi$ ,  $\epsilon$ , and the unknown value of  $\alpha_{\text{ex}}$  are determined from the four values  $\alpha_0, \dots, \alpha_3$ , with the result

$$\eta = 2.529298, \quad \xi = 0.660946, \quad \epsilon = 1.976207, \quad (4.2)$$

and the extrapolated value for the exact constant:

$$\alpha_{\text{ex}} = 0.0797149. \quad (4.3)$$

This is now in perfect agreement with the Monte Carlo values (1.3).

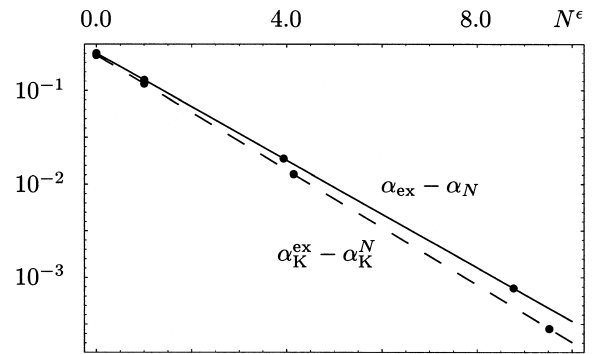


Fig. 1. Difference between the extrapolated pressure constant  $\alpha_{\text{ex}}$  and the optimized  $N$ -th order value  $\alpha_N$  obtained from variational perturbation theory for the method presented in this paper (solid line) and the first four values of the approximation scheme introduced in Ref. [4] (dashed line). Dots represent the values to order  $N$  in these approximations.

The approach is graphically shown in Fig. 1 where the optimized values  $\alpha_0, \dots, \alpha_3$  all lie on a straight line (solid line). For comparison, we have also extrapolated the first four values  $\alpha_K^0, \dots, \alpha_K^3$  in the approach of Ref. [4] yielding a value  $\alpha_{\text{exK}} \approx 0.0759786$ , which is 4.9% smaller than (4.3).

#### 5. Summary

We have calculated the universal constant  $\alpha$  occurring in the pressure law (1.1) of a membrane fluctuating between two walls. This has been done by replacing the walls by a smooth potential with a parameter  $m^2$ . This potential approaches the wall potential in the limit  $m^2 \rightarrow 0$ . The anharmonic part of the smooth potential was treated perturbatively. The limit  $m^2 \rightarrow 0$  corresponds to a strong-coupling limit of the power series, and was calculated by variational perturbation theory. Extrapolating the lowest four approximations to infinity yields a pressure constant  $\alpha$ , which is in very good agreement with Monte Carlo values.

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