

# Derivation of the Spherical Harmonic Decomposition for Quasi-Spherical Vesicle Shapes

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## Abstract

This document provides a detailed and pedagogical derivation of how a quasi-spherical lipid vesicle shape can be expanded into spherical harmonics, starting from the equilibrium spherical configuration. We begin by introducing the Helfrich free energy model for lipid membranes, discuss the constraints of fixed volume and area, and motivate the use of spherical harmonics as a natural basis for small perturbations around a sphere. We show how these basis functions simplify the analysis of curvature, area, and volume changes, and highlight why particular modes (e.g.,  $\ell = 0$  and  $\ell = 1$ ) must vanish under physical constraints. This detailed exposition is intended to give a full understanding of the steps commonly cited in the literature on membrane fluctuations and vesicle shape analysis.

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# 1 Introduction

Lipid vesicles are closed membranes composed of lipid bilayers, often approximated as two-dimensional fluid surfaces embedded in three-dimensional space. Their equilibrium shape results from the competition between bending energy, tension, and volume (or pressure) constraints. A widely used theoretical description for the energy of a vesicle is given by the Helfrich free energy functional [1–3].

At mechanical equilibrium, in the absence of external forces, a vesicle often adopts a simple spherical shape. However, thermal fluctuations, external fields, or chemical signals can induce small deviations from perfect sphericity. To systematically analyze these small perturbations, it is natural to choose a complete orthonormal basis defined on the sphere. The standard choice is the set of spherical harmonics  $Y_{\ell m}(\theta, \phi)$ .

In this document, we start from an equilibrium spherical shape of radius  $R_0$ , introduce a small shape perturbation, and then decompose this perturbation into spherical harmonics. We will also discuss how constraints like fixed volume and fixed area translate into conditions on these spherical harmonic modes.

# 2 Helfrich Energy and Constraints

## 2.1 Helfrich Energy Functional

The Helfrich energy [1] for a closed vesicle without spontaneous curvature can be written as:

$$E = \frac{\kappa}{2} \int (2H)^2 dA + \sigma \int dA + \Delta p \int dV, \quad (1)$$

where

- $\kappa$  is the bending rigidity.
- $H$  is the mean curvature of the membrane surface.
- $\sigma$  is the surface tension.
- $\Delta p$  is the pressure difference between the inside and outside of the vesicle.
- $dA$  is the surface element.
- $dV$  is the volume element enclosed by the membrane.

For a sphere of radius  $R_0$ , the mean curvature is constant,  $H = 1/(2R_0)$ , and the equilibrium energy has contributions from bending, tension, and the pressure-volume term. At equilibrium,  $R_0$  is determined by balancing these terms under the constraints of fixed total area  $A_0 = 4\pi R_0^2$  and fixed volume  $V_0 = \frac{4}{3}\pi R_0^3$ .

## 2.2 Volume and Area Constraints

In most physical situations:

1. The volume  $V$  enclosed by the membrane is essentially fixed due to incompressibility of the internal fluid.
2. The area  $A$  of the membrane is also approximately fixed because it is very costly to stretch a lipid bilayer.

Thus, we have  $A = A_0$  and  $V = V_0$  to a very good approximation. Small deviations from the equilibrium shape must respect (or nearly respect) these constraints:

$$\Delta V \approx 0, \quad \Delta A \approx 0. \quad (2)$$

These constraints will lead to conditions on the spherical harmonic coefficients, as we will see below.

## 3 Parameterizing the Vesicle Shape

### 3.1 Equilibrium Spherical Shape

Consider a coordinate system  $(r, \theta, \phi)$  where  $\theta$  is the polar angle ( $0 \leq \theta \leq \pi$ ) and  $\phi$  is the azimuthal angle ( $0 \leq \phi < 2\pi$ ). For a perfect sphere of radius  $R_0$ , every point on the surface is given by:

$$\mathbf{r}_0(\theta, \phi) = R_0 \hat{\mathbf{r}}(\theta, \phi), \quad (3)$$

where  $\hat{\mathbf{r}}(\theta, \phi)$  is the unit vector in the radial direction.

### 3.2 Perturbed Shape

We now consider a small deviation from the spherical shape. Let  $R(\theta, \phi)$  be the radial distance of the vesicle surface from the center in the direction  $(\theta, \phi)$ :

$$R(\theta, \phi) = R_0 [1 + u(\theta, \phi)], \quad (4)$$

where  $|u(\theta, \phi)| \ll 1$  ensures we are dealing with small perturbations. The dimensionless function  $u(\theta, \phi)$  represents how much the radius deviates from  $R_0$  in each angular direction.

## 4 Spherical Harmonics Expansion

### 4.1 Motivation for Spherical Harmonics

On a sphere, the natural generalization of Fourier modes (which are used on a line or a circle) are spherical harmonics  $Y_{\ell m}(\theta, \phi)$  [6, 7]. These functions form an orthonormal and complete basis for expansions of scalar functions defined on the sphere.

Any sufficiently smooth function  $f(\theta, \phi)$  can be expanded as:

$$f(\theta, \phi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} f_{\ell m} Y_{\ell m}(\theta, \phi). \quad (5)$$

The  $Y_{\ell m}$  are defined as:

$$Y_{\ell m}(\theta, \phi) = N_{\ell m} P_{\ell}^m(\cos \theta) e^{im\phi}, \quad (6)$$

where  $P_{\ell}^m$  are the associated Legendre polynomials and  $N_{\ell m}$  is a normalization constant such that:

$$\int_0^{2\pi} \int_0^{\pi} Y_{\ell m}(\theta, \phi) Y_{\ell' m'}^*(\theta, \phi) \sin \theta d\theta d\phi = \delta_{\ell\ell'} \delta_{mm'}. \quad (7)$$

Spherical harmonics diagonalize angular momentum operators and are eigenfunctions of the spherical Laplacian. This makes them extremely convenient for analyzing curvature-related quantities on the vesicle.

## 4.2 Expanding $u(\theta, \phi)$

We now expand the perturbation  $u(\theta, \phi)$  in terms of spherical harmonics:

$$u(\theta, \phi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} u_{\ell m} Y_{\ell m}(\theta, \phi). \quad (8)$$

Thus, the full vesicle radius can be written as:

$$R(\theta, \phi) = R_0 \left[ 1 + \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} u_{\ell m} Y_{\ell m}(\theta, \phi) \right]. \quad (9)$$

Each pair  $(\ell, m)$  represents a particular angular mode of deformation. Modes with low  $\ell$  correspond to large-scale, low-frequency deformations, while high  $\ell$  modes represent more intricate shape fluctuations.

# 5 Volume and Area Constraints in Terms of Spherical Harmonics

## 5.1 Volume Constraint

The volume enclosed by the vesicle is:

$$V = \int_{\text{inside surface}} dV. \quad (10)$$

For a nearly spherical shape:

$$V \approx \frac{4\pi R_0^3}{3} [1 + 3\langle u(\theta, \phi) \rangle_{\Omega}], \quad (11)$$

to first order in  $u$ , where  $\langle \dots \rangle_{\Omega}$  denotes the average over the solid angle:

$$\langle u(\theta, \phi) \rangle_{\Omega} = \frac{1}{4\pi} \int_0^{2\pi} \int_0^{\pi} u(\theta, \phi) \sin \theta d\theta d\phi. \quad (12)$$

Inserting the spherical harmonic expansion:

$$u(\theta, \phi) = \sum_{\ell, m} u_{\ell m} Y_{\ell m}(\theta, \phi), \quad (13)$$

and using the orthogonality of  $Y_{\ell m}$ , we recall that:

$$Y_{00}(\theta, \phi) = \frac{1}{\sqrt{4\pi}}. \quad (14)$$

Hence,

$$\langle u(\theta, \phi) \rangle_{\Omega} = \sum_{\ell, m} u_{\ell m} \frac{1}{4\pi} \int_0^{2\pi} \int_0^{\pi} Y_{\ell m}(\theta, \phi) \sin \theta \, d\theta \, d\phi. \quad (15)$$

All integrals vanish except for  $\ell = 0, m = 0$ . For  $\ell = 0, m = 0$ :

$$\int_0^{2\pi} \int_0^{\pi} Y_{00}(\theta, \phi) \sin \theta \, d\theta \, d\phi = \int_0^{2\pi} \int_0^{\pi} \frac{1}{\sqrt{4\pi}} \sin \theta \, d\theta \, d\phi. \quad (16)$$

First integrate over  $\phi$ :

$$\int_0^{2\pi} d\phi = 2\pi.$$

Then integrate over  $\theta$ :

$$\int_0^{\pi} \sin \theta \, d\theta = 2.$$

Thus:

$$\int_0^{2\pi} \int_0^{\pi} Y_{00} \sin \theta \, d\theta \, d\phi = \frac{1}{\sqrt{4\pi}} (2\pi)(2) = \frac{4\pi}{\sqrt{4\pi}} = 2\sqrt{\pi}. \quad (17)$$

Since we have a factor  $1/(4\pi)$  in the average, we get:

$$\langle u(\theta, \phi) \rangle_{\Omega} = \frac{u_{00}}{4\pi} (2\sqrt{\pi}) = \frac{u_{00}}{2\sqrt{\pi}}. \quad (18)$$

The volume to first order in  $u$  is:

$$V \approx V_0(1 + 3\langle u \rangle_{\Omega}) = V_0 \left( 1 + \frac{3u_{00}}{2\sqrt{\pi}} \right). \quad (19)$$

If volume is to remain constant,  $\Delta V = 0$ , we must have:

$$3\langle u \rangle_{\Omega} = 0 \implies u_{00} = 0. \quad (20)$$

This condition means there can be no net monopole expansion or contraction of the vesicle radius. Physically,  $u_{00}$  represents a uniform rescaling of the radius, changing the volume. With volume fixed, this mode is forbidden.

## 5.2 Area Constraint

A similar calculation applies to the area:

$$A = \int_0^{2\pi} \int_0^{\pi} R(\theta, \phi)^2 \sin \theta \, d\theta \, d\phi. \quad (21)$$

Since  $R(\theta, \phi) = R_0[1 + u(\theta, \phi)]$ , to first order:

$$R(\theta, \phi)^2 \approx R_0^2(1 + 2u(\theta, \phi)). \quad (22)$$

Thus,

$$A \approx 4\pi R_0^2 (1 + 2\langle u(\theta, \phi) \rangle_{\Omega}). \quad (23)$$

For  $A = A_0 = 4\pi R_0^2$  to hold, we again need  $\langle u(\theta, \phi) \rangle_{\Omega} = 0$ , reinforcing the  $u_{00} = 0$  condition under a strict area constraint. More subtle constraints might redistribute conditions among other modes, but typically  $u_{00} = 0$  suffices if both volume and area are fixed.

## 6 Eliminating Translational Modes

Consider the  $\ell = 1$  modes. The  $\ell = 1$  spherical harmonics correspond essentially to dipolar distortions of the shape:

$$Y_{10}(\theta, \phi) \sim \cos \theta, \quad Y_{1,\pm 1}(\theta, \phi) \sim \sin \theta e^{\pm i\phi}.$$

A perturbation in the  $\ell = 1$  modes can be interpreted as shifting the center of the sphere along some direction i.e., translating the vesicle without changing its shape. Such a translation does not alter the bending energy associated with shape deformations, nor does it contribute to volume or area changes in a meaningful way distinct from changing coordinates.

By choosing our coordinate system such that the center of the vesicle remains fixed at the origin, we can set:

$$u_{1m} = 0 \quad \text{for } m = -1, 0, 1. \quad (24)$$

This removes spurious translational modes and ensures that all remaining modes ( $\ell \geq 2$ ) correspond to genuine shape deformations.

## 7 Helfrich Energy Expansion in Spherical Harmonics

Once we have the shape expanded in spherical harmonics and have enforced  $u_{00} = 0$  and  $u_{1m} = 0$ , the Helfrich energy can be expanded in terms of  $u_{\ell m}$ . The mean curvature  $H$  and the area element  $dA$  can be expanded for small  $u_{\ell m}$ , leading to an energy expression:

$$E = E_0 + \sum_{\ell=2}^{\infty} \sum_{m=-\ell}^{\ell} E_{\ell m}(u_{\ell m}, \kappa, \sigma, \Delta p, R_0), \quad (25)$$

where  $E_0$  is the energy of the perfect sphere. Each mode  $(\ell, m)$  can often be analyzed separately due to orthogonality, and one obtains effective potentials that govern the amplitude of these modes. Minimizing this energy subject to volume and area constraints gives equilibrium shape fluctuations and their spectra.

This decomposition is the basis for studying thermal fluctuations of membranes, instabilities induced by changes in tension or pressure, and more complex phenomena where the shape responds to chemical gradients or other environmental cues.

## 8 Summary and Conclusions

We began with the equilibrium spherical vesicle shape and introduced a small perturbation to the radius. By expanding this perturbation in spherical harmonics, we leveraged their orthogonality and completeness to decompose complicated shape variations into well-defined angular modes. We found that:

- The  $\ell = 0$  mode (monopole) corresponds to uniform radius changes. For fixed volume and area,  $u_{00} = 0$  must hold.
- The  $\ell = 1$  modes correspond to translations. By choosing the reference frame at the vesicles center, we can set  $u_{1m} = 0$ .

- The remaining modes  $\ell \geq 2$  represent genuine shape deformations that can be analyzed using the Helfrich energy framework.

This approach provides a natural, mathematically consistent way to analyze shape fluctuations of quasi-spherical vesicles. It is widely used in the literature of membrane biophysics and soft matter physics [2, 4, 5].

## 8.1 Expanding the Free Energy in Spherical Harmonics: The Spherical Analog of a Fourier Transform

In standard Fourier analysis, a function defined on a line or a circle can be expanded as an integral or a series of sines and cosines (or complex exponentials), leveraging the completeness and orthogonality of these basis functions. For functions defined on the surface of a sphere, the corresponding natural basis functions are the spherical harmonics. In this subsection, we outline the mathematical reasoning that expanding the vesicle free energy in spherical harmonics is the spherical analog of performing a Fourier decomposition.

**Step 1: Completeness and Orthonormality of Spherical Harmonics.** Consider the unit sphere  $S^2$  parameterized by the angles  $\theta \in [0, \pi]$  and  $\phi \in [0, 2\pi)$ . The spherical harmonics  $Y_{\ell m}(\theta, \phi)$  are eigenfunctions of the angular part of the Laplacian operator on the sphere. For each integer  $\ell \geq 0$  and  $m$  such that  $-\ell \leq m \leq \ell$ , the spherical harmonic  $Y_{\ell m}$  is defined as:

$$Y_{\ell m}(\theta, \phi) = N_{\ell m} P_{\ell}^m(\cos \theta) e^{im\phi}, \quad (26)$$

where  $P_{\ell}^m$  are the associated Legendre polynomials and  $N_{\ell m}$  is a normalization constant.

The key properties we use are: 1. *Orthonormality*:

$$\int_0^{2\pi} \int_0^{\pi} Y_{\ell m}(\theta, \phi) Y_{\ell' m'}^*(\theta, \phi) \sin \theta d\theta d\phi = \delta_{\ell\ell'} \delta_{mm'}, \quad (27)$$

where the asterisk denotes complex conjugation and  $\delta$  is the Kronecker delta.

2. *Completeness*: Any square-integrable function  $f(\theta, \phi)$  defined on the sphere can be expanded as:

$$f(\theta, \phi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} f_{\ell m} Y_{\ell m}(\theta, \phi), \quad (28)$$

where the expansion coefficients are given by:

$$f_{\ell m} = \int_0^{2\pi} \int_0^{\pi} f(\theta, \phi) Y_{\ell m}^*(\theta, \phi) \sin \theta d\theta d\phi. \quad (29)$$

These properties directly parallel those of the exponential basis  $e^{ikx}$  on a line or the sine and cosine basis on a circle, but adapted to the geometry of a sphere.

**Step 2: Applying to the Vesicle Perturbation Field.** We consider a vesicle with a shape characterized by a radial function:

$$R(\theta, \phi, t) = R_0[1 + u(\theta, \phi, t)], \quad (30)$$

where  $u(\theta, \phi, t)$  is a small dimensionless perturbation that may depend on time  $t$ . Since  $u(\theta, \phi, t)$  is a function defined on the unit sphere (for each fixed time  $t$ ), we can expand it in spherical harmonics:

$$u(\theta, \phi, t) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} u_{\ell m}(t) Y_{\ell m}(\theta, \phi). \quad (31)$$

This decomposition is the spherical analog of writing a function  $f(x)$  as a Fourier series  $f(x) = \sum_k f_k e^{ikx}$ , except now the "wavenumbers"  $k$  are replaced by the angular quantum numbers  $(\ell, m)$ , and the exponential functions are replaced by  $Y_{\ell m}$ .

**Step 3: Substitution into the Free Energy.** The Helfrich free energy of the membrane can be expressed as:

$$F = \frac{\kappa}{2} \int (2H)^2 dA + \sigma \int dA + \Delta p \int dV. \quad (32)$$

Each of the geometric quantities  $(H, dA, dV)$  can be expanded in terms of the spherical harmonic modes of  $u(\theta, \phi, t)$ . Due to the orthogonality of  $Y_{\ell m}$ , when we integrate these quantities over the spherical angles, the cross-terms vanish. This leaves us with a free energy  $F$  expressed as a sum over independent  $(\ell, m)$  modes:

$$F = F_0 + \sum_{\ell, m} F_{\ell m}(u_{\ell m}(t)), \quad (33)$$

where  $F_0$  is the energy of the reference sphere and  $F_{\ell m}$  are contributions from each mode.

The orthogonality of spherical harmonics ensures that each  $(\ell, m)$  mode contributes separately, analogous to how a Fourier transform diagonalizes convolution operators or separates different wavenumbers in a flat geometry.

**Step 4: Interpreting the Expansion as a Spherical Fourier Transform.** In Cartesian spaces, performing a Fourier transform simplifies differential operators and decouples modes with different  $k$ -values. On a sphere, expanding in spherical harmonics serves the same purpose: it leverages the eigenfunction property of  $Y_{\ell m}$  under the spherical Laplacian and related geometric operators. Thus, analyzing the vesicle shape and its free energy in terms of spherical harmonics is functionally equivalent to performing a Fourier decomposition in the appropriate geometry (the 2D surface of a sphere).

**Conclusion.** While the standard Fourier transform is defined on infinite or periodic flat domains, the spherical harmonics provide a natural "Fourier-like" expansion for functions on the surface of a sphere. Thus, when we expand the vesicle free energy in spherical harmonics, we are essentially performing the spherical analog of a Fourier transform. This transforms the problem into one where each  $(\ell, m)$  mode can be treated independently, greatly simplifying analysis and providing clear physical interpretations of different deformation modes.

In summary: - Spherical harmonics form a complete, orthonormal set of functions on  $S^2$ . - Any function on the sphere, including the perturbation  $u(\theta, \phi, t)$ , can be expanded in these functions. - The expansion allows the free energy to be expressed as a sum of independent mode contributions, analogous to how a Fourier transform decomposes a function into independent frequency components.



## 8.2 Analogy with the Standard Fourier Transform

To understand why expanding the vesicle free energy in spherical harmonics is the spherical analog of a Fourier transform, it helps to recall the role of the Fourier transform in a simpler setting: a function defined on a line or a circle.

**Fourier Transform in Flat Space.** Consider a one-dimensional function  $f(x)$  defined for  $x \in (-\infty, \infty)$ . The standard Fourier transform  $\mathcal{F}$  maps  $f(x)$  into a function  $\hat{f}(k)$  defined on the wavevector (or frequency) domain:

$$\hat{f}(k) = \int_{-\infty}^{\infty} f(x) e^{-ikx} dx. \quad (34)$$

The inverse transform recovers  $f(x)$ :

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{f}(k) e^{ikx} dk. \quad (35)$$

If  $f(x)$  is periodic with period  $L$ , the integral transform is replaced by a Fourier series:

$$f(x) = \sum_{n=-\infty}^{\infty} f_n e^{i\frac{2\pi n}{L}x}, \quad \text{where } f_n = \frac{1}{L} \int_0^L f(x) e^{-i\frac{2\pi n}{L}x} dx. \quad (36)$$

These representations (the integral transform in infinite space and the Fourier series on a periodic domain) rest on the completeness and orthogonality of the exponential functions  $e^{ikx}$ .

**Fourier-Like Expansion on the Sphere.** On a 2D sphere  $S^2$ , we cannot use standard exponentials  $e^{ikx}$  directly because the domain is a curved surface without a global Cartesian coordinate  $x$ . Instead, the natural orthonormal basis for functions on  $S^2$  are the spherical harmonics  $Y_{\ell m}(\theta, \phi)$ .

Just as the exponential functions  $\{e^{ikx}\}$  form a complete orthonormal set on a line or circle, the spherical harmonics  $\{Y_{\ell m}\}$  form a complete orthonormal set on the sphere. Consequently, any function  $u(\theta, \phi)$  defined on the spherical surface can be decomposed as:

$$u(\theta, \phi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} u_{\ell m} Y_{\ell m}(\theta, \phi), \quad (37)$$

where the coefficients  $u_{\ell m}$  are obtained by integrating against the complex conjugate of  $Y_{\ell m}$ :

$$u_{\ell m} = \int_0^{2\pi} \int_0^{\pi} u(\theta, \phi) Y_{\ell m}^*(\theta, \phi) \sin \theta d\theta d\phi. \quad (38)$$

This is directly analogous to how  $f_n$  or  $\hat{f}(k)$  are obtained in the Fourier series or Fourier transform of  $f(x)$ , with the crucial difference that the geometry is now spherical rather than flat or periodic in one dimension.

**Applying This to the Free Energy.** For the vesicle problem, we start with a free energy functional like:

$$F = \frac{\kappa}{2} \int (2H)^2 dA + \sigma \int dA + \Delta p \int dV. \quad (39)$$

If we consider the shape perturbation  $u(\theta, \phi)$ , and insert its spherical harmonic expansion, the integrals over the spherical angles separate into sums over  $\ell, m$  due to the orthogonality of  $Y_{\ell m}$ . This leads to a mode-by-mode decomposition of the free energy, just as a Fourier transform would separate a function into its independent frequency components:

$$F = F_0 + \sum_{\ell, m} F_{\ell m}(u_{\ell m}). \quad (40)$$

Here, each  $(\ell, m)$  plays a role analogous to a wavenumber or frequency in the Fourier transform scenario. In one dimension,  $k$  labels different frequencies. On the sphere,  $(\ell, m)$  index different angular modes.

**Conceptual Equivalence.** - \*\*Fourier Transform on a Line/Circle:\*\* - Basis Functions:  $e^{ikx}$  or  $e^{i\frac{2\pi n}{L}x}$  - Decomposition:  $f(x) = \int dk \hat{f}(k)e^{ikx}$  or  $f(x) = \sum_n f_n e^{i\frac{2\pi n}{L}x}$  - Orthogonality:  $\int_0^L e^{i\frac{2\pi}{L}(n-n')x} dx \propto \delta_{nn'}$

- \*\*Spherical Harmonics on a Sphere:\*\* - Basis Functions:  $Y_{\ell m}(\theta, \phi)$  - Decomposition:  $u(\theta, \phi) = \sum_{\ell, m} u_{\ell m} Y_{\ell m}(\theta, \phi)$  - Orthogonality:  $\int_0^{2\pi} \int_0^\pi Y_{\ell m} Y_{\ell' m'}^* \sin \theta d\theta d\phi = \delta_{\ell\ell'} \delta_{mm'}$

In both cases, the expansion allows us to rewrite integrals and operators in a simpler, diagonalized form. The spherical harmonic expansion is thus the natural generalization of a Fourier transform to a spherical geometry.

**Conclusion.** In summary, although we do not typically call the spherical harmonic expansion a Fourier transform because the domain is a sphere and not a line or plane, the conceptual role is the same. Expanding a function in spherical harmonics is effectively performing a Fourier-like expansion tailored to the geometry of the sphere. Thus, analyzing the vesicles free energy in terms of spherical harmonics is the curved-surface equivalent of applying a Fourier transform in a flat domain.

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