Curvature-based interaction potential between a micro/nano curved surface body and a particle on the surface of the body

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Abstract The interaction potential between a curved surface body and a particle located on the surface of the body is studied in this paper. Based on the negative exponential pair potential ($1/R^n$) between particles, the interaction potential is proved to be of the curvature-based form, i.e., it can be written as a function of curvatures of the surface. Idealized numerical experiments are designed to test the accuracy of curvature-based potential. Based on the curvature-based potential, propositions below are confirmed: a highly curved surface body will induce driving forces on the particle located on the surface, and curvatures and the gradients of curvatures are essential factors forming the driving forces. In addition, the tangent driving force acting on the particle from the curved surface body is studied. Based on duality, the following rule is proved: for a convex or concave curved body sharing the same curved surface, the curvature-based interaction potential between them and a particle on the surface can make up the potential of a particle in the whole space.

Keywords Micro/nano curved surface body · Particle on the surface · Pair-potential · Curvature-based potential · Driving force of curvatures and the gradients of curvatures

1 Introduction

At micro/nano scales, molecules can move spontaneously on the surface of soft materials such as biomembranes. Such spontaneous movements can control the shape

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of soft materials and further change surface topography. For example, small particles on the surface of water will move spontaneously towards a hydrophilic cylinder that is vertically inserted in the water [1]. Phase separation of soft materials will occur spontaneously on a substrate with certain geometrical morphologies [2–4]. With high mobility of biomembranes, differentiation can occur for some cells, and when a cell becomes pathological, its shape will change greatly [5, 6]. To explain such phenomena, it is necessary to understand the interaction between a micro/nano curved surface body and the particle on the surface. Such study is also essential for elaborating fundamental concepts such as the surface tension in micro/nano mechanics. In fact, the surface tension of a liquid is the total interaction potential between a particle on the surface and all the other particles distributed on the surface and inside the liquid [7].

Recently, based on the negative exponential pair potential, Yin et al. [8] studied the interaction between a curved surface and a particle located outside the surface. Wu et al. [9, 10] discussed the interaction between a curved surface and a particle located on the surface. Wang et al. [11] investigated the potential of a curved line and a particle located outside the line. Later, the interaction potential of a curved surface body and an outside particle was studied by Wang et al. [12, 13]. All of this research verified that the interaction potential between a particle and a curved material space can be written as a function of curvatures. As materials are highly curved at micro/nano scales, the interaction potential of a particle on the surface is closely related to the surface topography, which can be depicted by curvatures directly.

Previously, the interaction between a curved surface body and a particle has been classified into three basic modes [13]: (I) the interaction between a curved surface body and a particle outside the body (Fig. 1a), (II) the interaction between a curved surface body and a particle on the surface of the body (Fig. 1b), (III) the interaction between a curved surface body and a particle inside the body (Fig. 1c). Mode (I) has been studied and the interaction potential between a curved surface body and an outside particle has been proven to be a function of curvatures [12, 13]. However, the topological structures of the three modes have intrinsic differences. When a particle is located outside a curved surface body (Fig. 1a), the characteristic parameter is h . For the particle on the surface of curved surface body (Fig. 1b), it will occupy a certain area because of the strong repulsive force when two particles are close enough; we assume the radius of this area is given by the characteristic parameter τ . For a particle inside a curved surface body (Fig. 1c), the characteristic parameters are h and τ . From the viewpoint of physics and mechanics, once topology changes, the physical and mechanical properties will also change. The three modes correspond to different topologies, and should be studied separately. Particularly, it is noted that the mode (II) is not the limitation of the mode (I) when $h \rightarrow 0$. Actually, previous research has indicated that the mode (I) corresponds to a singularity when $h \rightarrow 0$, which is a physically high energy barrier [12, 13].

Though the three modes have explicit differences, they also have apparent relations. As they are all related to the interaction between a curved surface body and a particle, the methods and approaches of the studies are similar.

This paper will focus on mode (II), and answer the question of whether the interaction potential between a curved surface body and a particle on the surface can be written in a curvature-based form.

Fig. 1 **a** Interaction between a curved surface body and an outside particle. **b** Interaction between a curved surface body and a particle on the surface. **c** Interaction between a curved surface body and an inside particle

2 Interaction between semi-infinite plane body and on-surface particle

Firstly, the interaction between a semi-infinite plane body and a particle P on the surface of a plane is recalled. As shown in Fig. 2, the pair potential between particles is taken as $u(r)=C/r^n$ [14], which is the abstracted form of the L-J potential $u(r)=\varepsilon[(\sigma/r)^{12}-(\sigma/r)^6]$.

At small scales, there are different kinds of pair potentials between particles and $u(r)=C/r^n$ is just one of the most widely used. Later, we will study other interaction pair potentials such as $u(r)=Ce^{-r/\lambda}$ and will prove that the curvature-based potential is still available.

The number density of molecules in the semi-infinite plane body is ρ and the equivalent radius of particle P on the surface is τ . Then the interaction potential between a semi-infinite plane body and the particle P is:

$$\overline{U}(\tau) = \frac{2\pi\rho C}{(n-3)\tau^{n-3}} \quad n \geq 4 \quad (1)$$

Fig. 2 Interaction between semi-infinite plane body and a particle on the surface

3 Further classification and approximation of the local shape of a curved surface body

In previous research [13], we have classified a curved surface body and approximated the local shape. Here we directly use the previous result. According to the bending direction, curved surface bodies are divided into two categories, i.e., convex curved surface bodies (Fig. 3a) and concave curved surface bodies (Fig. 3b). This paper will not consider the curved surface body with negative Gaussian curvature, such as the saddle curved surface body.

As shown in Figs. 4 and 5, a unified orthogonal coordinate system $P\text{-}xyz$ is built with the origin at P . The positive direction of the z -axis always points to the concave side of the outer surface S of the curved surface body V . The xy plane is the tangent plane of the outer surface S at the point P . Axes x and y coincide with the tangent direction of the principal curvature lines, respectively.

Because the pair potential between particles is of very short range, the effective zone on the curved surface body interacting with particle P mainly covers the neighborhood V_δ of the particle P . The function of the curved surface S can be written as $z=f(x,y)$ in the local coordinate system $P\text{-}xyz$. According to differential geometry [14], the first-order partial derivatives of the function $z=f(x,y)$ at point P are zero, i.e., $f(0,0)=0$, $f_x(0,0)=0$, $f_y(0,0)=0$. Similar to previous research [8–10, 12, 13], $f(x,y)$ can be expanded with a Taylor series to the second order at point P :

$$z = f(x,y) \approx \frac{1}{2} (f_{xx}^0 x^2 + f_{yy}^0 y^2) \quad (2)$$

Fig. 3 **a** Interaction between convex curved surface body and a particle located on the surface of the body. **b** Interaction between a concave curved surface body and a particle located on the surface of the body

Fig. 4 Schematic figure of the interaction between a convex curved surface body and an on-surface particle. **a** A 3D diagram of the interaction between a convex curved surface body and an on-surface particle. **b** A 2D diagram of the interaction between a convex curved surface body and an on-surface particle

Equation (2) is a quadric surface, which may be marked as S_0 . The curved surface body V_0 with the quadric outer surface S_0 is used to approximate the original body V . Here f_{xx}^0 and f_{yy}^0 are the second partial derivatives of S_0 at point P . Under the principle curvature coordinate system, they determine the two principle curvatures:

$$c_1 = f_{xx}^0, \quad c_2 = f_{yy}^0 \quad (3)$$

Substituting Eq. (3) into Eq. (2) will lead to the function of local shape of S_0 :

$$z = \frac{1}{2}(c_1 x^2 + c_2 y^2) \quad (4)$$

In the coordinate system shown in Figs. 4 and 5, we have $c_1 > 0$ and $c_2 > 0$, and the relationship between the original curved surface body V and the approximate curved surface body V_0 is shown in Fig. 6.

Fig. 5 Schematic figure of the interaction between a concave curved surface body and an on-surface particle. **a** A 3D diagram of the interaction between a concave curved surface body and an on-surface particle. **b** A 2D diagram of the interaction between a concave curved surface body and an on-surface particle

Fig. 6 Relationship between a curved surface body and a quadric curved surface body

4 Interaction potential between a curved surface body and a particle on the surface of the body

In this section, we will study the interaction potential between a curved surface body V_0 and the particle P on S_0 .

4.1 General formulation of the interaction potential

The particle P on S_0 interacts with other particles both on S_0 and inside V_0 . Thus, the interaction between particle P and V_0 is a volume integral. If we draw a spherical shell S_P with the center at particle P and radius R , then the intersection of V_0 and S_P is an arc surface. The area of S_P is marked as A . If the spherical shell has thickness dR , then the volume of the intersected body is AdR . The total number of particles inside the volume is ρAdR . The interaction potential between particle P and curved surface body V_0 is:

$$U_n = \int_{\tau}^{\infty} \frac{C\rho A}{R^n} dR \quad (5)$$

Equation (5) is valid for both convex and concave surface bodies.

4.2 The unified formulation of the area of arc surface

In order to derive the area A of the arc surface S_P in Eq. (5), a cylindrical coordinate system $P-r\theta z$ with point P as the pole and axis x as the polar axis is established. The following transformation is established:

$$x = r\cos\theta, \quad y = r\sin\theta \quad (6)$$

Substituting Eq. (6) into Eq. (4), we get:

$$z = \frac{1}{2} (c_1 \cos^2\theta + c_2 \sin^2\theta) r^2 = \frac{1}{2} k_n r^2 \quad (7)$$

Here:

$$k_n = c_1 \cos^2\theta + c_2 \sin^2\theta = \frac{1}{2} [(c_1 + c_2) + (c_1 - c_2) \cos 2\theta] \quad (8)$$

According to differential geometry [15], k_n is the normal curvature at point P in the direction with angle θ .

Either for a convex surface or for a concave surface, in the triangle CBP ,

$$R_k^2 + z^2 = R^2 \quad (9)$$

Here $R_k = |\vec{CA}|$ (Figs. 4 and 5). Solving Eqs. (7) and (9) we get R_k :

$$R_k^2 = \frac{\sqrt{1 + 4(k_n R)^2} - 1}{2k_n^2} \quad (10)$$

For particles on A ,

$$z = \sqrt{R^2 - r^2}$$

Here, r is the distance between particles and the z -axis. Then the area (R) intersected by convex surface S_P is:

$$\begin{aligned} \widehat{A}(R) &= \int_0^{2\pi} d\theta \int_0^{R_k(\theta, c_1, c_2)} \sqrt{1 + \left(\frac{\partial z}{\partial r}\right)^2} r dr = \int_0^{2\pi} d\theta \int_0^{R_k(\theta, c_1, c_2)} \sqrt{1 + \left(\frac{-r}{\sqrt{R^2 - r^2}}\right)^2} r dr \\ &= \int_0^{2\pi} R \left(R - \sqrt{R^2 - R_k^2} \right) d\theta \end{aligned} \quad (11)$$

Substituting Eq. (10) into Eq. (11) will give:

$$\begin{aligned} \widehat{A}(R) &= \int_0^{2\pi} R \left(R - \sqrt{R^2 - \frac{\sqrt{1 + 4(k_n R)^2 - 1}}{2k_n}} \right) d\theta \\ &= \int_0^{2\pi} R \left(R - \sqrt{\frac{4(Rk_n)^2 + 1 - 2\sqrt{4(Rk_n)^2 + 1} + 1}{4k_n^2}} \right) d\theta \\ &= \int_0^{2\pi} R \left(R + \frac{1}{2k_n} - \frac{1}{2k_n} \sqrt{4(Rk_n)^2 + 1} \right) d\theta \end{aligned} \quad (12)$$

The area $\widetilde{A}(R)$ intersected by concave S_P is:

$$\begin{aligned} \widetilde{A}(R) &= 4\pi R^2 - \int_0^{2\pi} d\theta \int_0^{R_k(\theta, c_1, c_2)} \sqrt{1 + \left(\frac{\partial z}{\partial r}\right)^2} r dr \\ &= 4\pi R^2 - \int_0^{2\pi} d\theta \int_0^{R_k(\theta, c_1, c_2)} \sqrt{1 + \left(\frac{-r}{\sqrt{R^2 - r^2}}\right)^2} r dr \\ &= \int_0^{2\pi} R \left(R + \sqrt{R^2 - R_k^2} \right) d\theta \end{aligned} \quad (13)$$

Substituting Eq. (10) into Eq. (13) will lead to:

$$\begin{aligned} \widetilde{A}(R) &= \int_0^{2\pi} R \left(R + \sqrt{R^2 - \frac{\sqrt{1 + 4(k_n R)^2 - 1}}{2k_n}} \right) d\theta \\ &= \int_0^{2\pi} R \left(R - \frac{1}{2k_n} + \frac{1}{2k_n} \sqrt{4(Rk_n)^2 + 1} \right) d\theta \end{aligned} \quad (14)$$

We define λ as:

$$\lambda = \begin{cases} -1 & \text{for convex curved surface body} \\ +1 & \text{for concave curved surface body} \end{cases} \quad (15)$$

Equations (12) and (14) can then be unified as:

$$A(R) = \int_0^{2\pi} R \left(R - \frac{\lambda}{2k_n} + \frac{\lambda}{2k_n} \sqrt{4(Rk_n)^2 + 1} \right) d\theta \quad (16)$$

4.3 Curvature-based interaction potential

Substituting Eq. (16) into Eq. (5) to get the unified interaction potential between the particle P and V_0 :

$$U_n = \int_{\tau}^{\infty} \int_0^{2\pi} \frac{C\rho}{R^{n-1}} \left(R - \frac{\lambda}{2k_n} + \frac{\lambda}{2k_n} \sqrt{4(Rk_n)^2 + 1} \right) d\theta dR \quad (17)$$

Here k_n is a function of curvatures c_1, c_2 . The purpose of this paper is to write Eq. (17) as an explicit formula of curvatures, with the aid of the method of the series expansion of small parametric variables [16]. The equivalent radius τ of the particle P is used as the characteristic length to define the dimensionless variables R and k_n :

$$\tilde{R} = \frac{R}{\tau}, \quad \tilde{k}_n = k_n \cdot \tau \quad (18)$$

Equation (17) can be rewritten as:

$$U_n = \frac{C\rho}{\tau^{n-3}} \int_1^{\infty} \int_0^{2\pi} \frac{1}{\tilde{R}^{n-1}} \left(\tilde{R} - \frac{\lambda}{2\tilde{k}_n} + \frac{\lambda}{2\tilde{k}_n} \sqrt{4(\tilde{R}\tilde{k}_n)^2 + 1} \right) d\theta d\tilde{R} \quad (19)$$

In Eq. (19), let:

$$f(\tilde{k}_n) = \sqrt{4(\tilde{R}\tilde{k}_n)^2 + 1} \quad (20)$$

Here $f(\tilde{k}_n)$ is a continuous and differentiable function of $\tilde{k}_n$. From Eqs. (8) and (18),

$$\begin{aligned} \tilde{k}_n &= \frac{1}{2} \tau \cdot [(c_1 + c_2) + (c_1 - c_2) \cos 2\theta] = \frac{1}{2} [(\tau \cdot c_1 + \tau \cdot c_2) + (\tau \cdot c_1 - \tau \cdot c_2) \cos 2\theta] \\ &= \frac{1}{2} [(\tilde{c}_1 + \tilde{c}_2) + (\tilde{c}_1 - \tilde{c}_2) \cos 2\theta] \end{aligned} \quad (21)$$

In the physical model, we consider that the equivalent radius τ is a small quantity compared to the curvature radius at point P , so that

$$\tilde{c}_1 \ll 1 \quad \tilde{c}_2 \ll 1 \quad (22)$$

From Eq. (21), $\tilde{k}_n$ is also a small quantity, i.e., $\tilde{k}_n \ll 1$. We take $\tilde{k}_n$ as the small parametric variable to use the series expansion [16]. $f(\tilde{k}_n)$ can be expanded as Taylor's series in $\tilde{k}_n$:

$$\begin{aligned}
f(\tilde{k}_n) \approx & f(0) + \left(\frac{\partial f}{\partial \tilde{k}_n} \bigg|_{\tilde{k}_n=0} \right) \tilde{k}_n + \frac{1}{2!} \left(\frac{\partial^2 f}{\partial \tilde{k}_n^2} \bigg|_{\tilde{k}_n=0} \right) \tilde{k}_n^2 + \frac{1}{3!} \left(\frac{\partial^3 f}{\partial \tilde{k}_n^3} \bigg|_{\tilde{k}_n=0} \right) \tilde{k}_n^3 \\
& + \frac{1}{4!} \left(\frac{\partial^4 f}{\partial \tilde{k}_n^4} \bigg|_{\tilde{k}_n=0} \right) \tilde{k}_n^4 + \cdots + \frac{1}{m!} \left(\frac{\partial^m f}{\partial \tilde{k}_n^m} \bigg|_{\tilde{k}_n=0} \right) \tilde{k}_n^m + O(\tilde{k}_n^m)
\end{aligned} \quad (23)$$

For simplification, we omit terms with orders higher than $(\hat{k}_n)^3$ obtain a polynomial function of the independent variable $\hat{k}_n$:

$$\begin{aligned}
f(\tilde{k}_n) &= f(0) + f'(0)\tilde{k}_n + \frac{f''(0)}{2!}\tilde{k}_n^2 + \frac{f'''(0)}{3!}\tilde{k}_n^3 + \frac{f^{(4)}(0)}{4!}\tilde{k}_n^4 + O(\tilde{k}_n^4) \\
&= 1 + 2\tilde{R}^2\tilde{k}_n^2 - 2\tilde{R}^4\tilde{k}_n^4
\end{aligned} \quad (24)$$

Substituting Eq. (24) into Eq. (19) gives:

$$U_n = \frac{C\rho}{\tau^{n-3}} \int_1^\infty \int_0^{2\pi} \frac{1}{\tilde{R}^{n-1}} \left[\tilde{R} + \lambda(\tilde{R}^2\tilde{k}_n - \tilde{R}^4\tilde{k}_n^3) \right] d\theta d\tilde{R} \quad (25)$$

Substituting Eq. (21) into Eq. (25) will lead to the terms below:

$$\begin{aligned}
\int_0^{2\pi} \tilde{k}_n d\theta &= \int_0^{2\pi} \frac{1}{2} \left[(\tilde{c}_1 + \tilde{c}_2) + (\tilde{c}_1 - \tilde{c}_2) \cos 2\theta \right] d\theta = \pi (\tilde{c}_1 + \tilde{c}_2) \int_0^{2\pi} \tilde{k}_n^3 d\theta \\
&= \int_0^{2\pi} \frac{1}{8} \left[(\tilde{c}_1 + \tilde{c}_2) + (\tilde{c}_1 - \tilde{c}_2) \cos 2\theta \right]^3 d\theta \\
&= \frac{\pi}{4} (\tilde{c}_1 + \tilde{c}_2)^3 + \frac{3\pi}{8} (\tilde{c}_1 + \tilde{c}_2) (\tilde{c}_1 - \tilde{c}_2)^2
\end{aligned} \quad (26)$$

According to differential geometry [15], the dimensionless mean curvature $\tilde{H}$ and Gaussian curvature $\tilde{K}$ are related to the principal curvatures $\tilde{c}_1$ and $\tilde{c}_2$ as follows:

$$\tilde{H} = \frac{1}{2} (\tilde{c}_1 + \tilde{c}_2), \quad \tilde{K} = \tilde{c}_1 \tilde{c}_2 \quad (27)$$

Substituting Eqs. (1), (26) and (27) into Eq. (25) leads to the interaction potential below:

$$U_n = \bar{U}_n \left[1 + \frac{n-3}{n-4} (\lambda \tilde{H}) - \frac{1}{2} \cdot \frac{n-3}{n-6} (\lambda \tilde{H}) (5\tilde{H}^2 - 3\tilde{K}) \right] \quad n > 6 \quad (28)$$

Here, $\bar{U}_n$ is the interaction potential between semi-infinite body and particle on the surface which is discussed in section 2. Equation (28) requires $n > 6$, which is related to the orders of $\tilde{k}_n$. If the function in Eq. (24) is only expanded to the second order of $\tilde{k}_n$, Eqs. (24) and (25) are rewritten as:

$$f(\tilde{k}_n) = f(0) + f'(0)\tilde{k}_n + \frac{f''(0)}{2!}\tilde{k}_n^2 + O(\tilde{k}_n^2) = 1 + 2\tilde{R}^2\tilde{k}_n^2$$

$$U_n = \frac{C\rho}{\tau^{n-3}} \int_1^\infty \int_0^{2\pi} \frac{1}{\tilde{R}^{n-1}} \left(\tilde{R} + \lambda \tilde{R}^2 \tilde{k}_n \right) d\theta d\tilde{R}$$

Then the interaction potential between the particle P and V_0 is:

$$U_n = \bar{U}_n \left[1 + \frac{n-3}{n-4} \left(\lambda \tilde{H} \right) \right] \quad n > 4 \quad (29)$$

In Eq. (29), the curvature-based potential is only affected by the mean curvature H . The lower requirement for index n provides wider practicability. The accuracy of Eqs. (28) and (29) will be tested in the section below.

Equation (28) indicates that U_n is affected largely by the local shape and topography of the surface S_0 . If the curved surface S_0 is flat enough, then the interaction potential U_n between V_0 and the particle P will degenerate to $\bar{U}_n$ between the semi-infinite plane body and the particle P . Once the planar surface is bent into a curved surface, the interaction potential is modified by two principal curvatures and can be written as the function of mean curvature H and Gaussian curvature K . The more curved the space is, the larger effect of curvatures will be. Thus, distribution of particles on the surface is closely related to surface morphology at micro/nano scales.

It should be noted that the condition in formulation (21) is very easy to be satisfied because the equivalent radius τ is usually much smaller than the principal radius of the curved surface. This means that the small parameter expansion method above is of universal application in micro/nano mechanics. In fact, in recent years, the small parameter expansion method has been successfully used to solve the problem of interaction potential between a curved surface or line and a particle [8–11], which has confirmed the universal applicability of the method.

5 Numerical verification

In the above curvature-based potential, two steps of approximations are included: one is that the general curved surface body V is replaced by the curved surface body V_0 . Another is the omitting of higher-order terms in the series expansion. As has been mentioned above, the interaction between particles is short range at micro/nano scales, thus particle P mainly interacts with the nearest zone V_δ on V . As V_0 approximates V_δ well, thus the first step of approximations are physically reasonable. Here we mainly focus on the influence of the second simplification.

Here, a numerical experiment is designed to verify the accuracy of the curvature-based potential. The curvature-based potential is not only related to curvatures but also influenced by the bending direction of the surface S_0 and the index n in the pair potential. Here we focus on the effect of curvature.

5.1 Accuracy of curvature-based potential in Eq. (28)

Firstly, both sides of the polynomial curvature-based potential (Eq. 28) are divided by $\bar{U}_n$ to get the dimensionless form:

$$\left(\tilde{U}_n\right)_{polynomial} = \frac{U_n}{\tilde{U}_n} = 1 + \frac{n-3}{n-4} \left(\lambda \tilde{H}\right) - \frac{1}{2} \cdot \frac{n-3}{n-6} \left(\lambda \tilde{H}\right) \left(5\tilde{H}^2 - 3\tilde{K}\right) \quad (30)$$

Then, both sides of Eq. (19) are divided by $\tilde{U}_n$ to get the dimensionless potential with integral form:

$$\left(\tilde{U}_n\right)_{numerical} = \frac{n-3}{2\pi} \int_1^\infty \int_0^{2\pi} \frac{1}{\tilde{R}^{n-1}} \left(\tilde{R} - \frac{\lambda}{2\tilde{k}_n} + \frac{\lambda}{2\tilde{k}_n} \sqrt{4\left(\tilde{R}\tilde{k}_n\right)^2 + 1} \right) d\theta d\tilde{R} \quad (31)$$

Here:

$$\tilde{k}_n = \frac{1}{2} \left[\left(\tilde{c}_1 + \tilde{c}_2 \right) + \left(\tilde{c}_1 - \tilde{c}_2 \right) \cos 2\theta \right] \quad (32)$$

Finally, by numerical calculation function *dblquad* in Matlab, $(\tilde{U}_n)_{numerical}$ in Eq. (31) can be obtained. $(\tilde{U}_n)_{numerical}$ and $(\tilde{U}_n)_{polynomial}$ in Eq. (30) are compared, and the accuracy may be estimated:

$$\delta = \left| \frac{\left(\tilde{U}_n\right)_{polynomial} - \left(\tilde{U}_n\right)_{numerical}}{\left(\tilde{U}_n\right)_{numerical}} \right| \quad (33)$$

In the following calculations, we will take $n=12$ and $n=6$, respectively. The accuracy of the curvature-based potential between convex V_0 and concave V_0 are listed in Tables 1 and 2,

Table 1 The error of curvature-based potential in Eq. (28) between a convex curved surface body and a particle ($n=12$)

$(\tilde{c}_1, \tilde{c}_2)$	$\left(\tilde{\tilde{U}}_{12}\right)_{numerical}$	$\left(\tilde{\tilde{U}}_{12}\right)_{numerical}$	$\delta(\times 100\%)$
(1/2, 0)	0.758159599023642	0.777343750000000	2.530357856191
(1/10, 0)	0.944213564203937	0.944218750000000	0.000549218552
(1/50, 0)	0.988751814047090	0.988753750000000	0.000195797659
(1/100, 0)	0.994372933741593	0.994375468750000	0.000254935379
(1/2, 1/2)	0.552870758442378	0.625000000000000	13.046311539578
(1/10, 1/10)	0.888970505843939	0.889000000000000	0.003317787921
(1/50, 1/50)	0.977510042702331	0.977512000000000	0.000200232998
(1/100, 1/100)	0.988748738346891	0.988751500000000	0.000279307877
(1/500, 1/500)	0.997749460084341	0.997750012000000	0.000055316057
(1/2, 1/10)	0.708165550635041	0.730000000000000	3.083240824886
(1/10, 1/50)	0.933034865745016	0.933040000000000	0.000550274719
(1/10, 1/100)	0.938619470752121	0.938625156250000	0.000605729804
(1/50, 1/100)	0.983128381097547	0.983130906250000	0.000256848699
(1/10, 1/500)	0.943094393391416	0.943099491250000	0.000540545954
(1/100, 1/500)	0.993248719543765	0.993250540000000	0.000183283018

Table 2 The error of curvature-based potential in Eq. (28) between a concave curved surface body and a particle ($n=12$)

$(\tilde{c}_1, \tilde{c}_2)$	$(\tilde{U}_{12})_{numerical}$	$(\tilde{U}_{12})_{polynomial}$	$\delta(\times 100\%)$
(1/2, 0)	1.241840400976359	1.222656250000000	1.544816142337
(1/10, 0)	1.055786435796063	1.055781250000000	0.000491178508
(1/50, 0)	1.011248185952910	1.011246250000000	0.000191441917
(1/100, 0)	1.005627066258407	1.005624531250000	0.000252082356
(1/2, 1/2)	1.447129241557622	1.375000000000000	4.984298533003
(1/10, 1/10)	1.111029494156061	1.111000000000000	0.002654669045
(1/50, 1/50)	1.022489957297669	1.022488000000000	0.000191424634
(1/100, 1/100)	1.011251261653109	1.011248500000000	0.000273092673
(1/500, 1/500)	1.002250539915659	1.002249988000000	0.000055067633
(1/2, 1/10)	1.291834449364959	1.270000000000000	1.690189433769
(1/10, 1/50)	1.066965134254984	1.066960000000000	0.000481201758
(1/10, 1/100)	1.061380529247879	1.061374843750000	0.000535670074
(1/50, 1/100)	1.016871618902453	1.016869093750000	0.000248325590
(1/10, 1/500)	1.056905606608584	1.056900508750000	0.000482338115
(1/100, 1/500)	1.006751280456234	1.006749460000000	0.000180824824

respectively, from which we can see that the curvature-based potential has enough accuracy when $\tilde{c}_1, \tilde{c}_2$ are small quantities.

Table 3 The error of curvature-based potential in Eq. (29) between a convex curved surface body and a particle ($n=6$)

$(\tilde{c}_1, \tilde{c}_2)$	$(\tilde{U}_{12})_{numerical}$	$(\tilde{U}_{12})_{numerical}$	$\delta(\times 100\%)$
(1/2, 0)	0.758159599023642	0.718750000000000	5.198061077693
(1/10, 0)	0.944213564203937	0.943750000000000	0.049095270552
(1/50, 0)	0.988751814047090	0.988750000000000	0.000183468396
(1/100, 0)	0.994372933741593	0.994375000000000	0.000207795118
(1/2, 1/2)	0.552870758442378	0.437500000000000	20.867581922295
(1/10, 1/10)	0.888970505843939	0.887500000000000	0.165416719033
(1/50, 1/50)	0.977510042702331	0.977500000000000	0.001027375873
(1/100, 1/100)	0.988748738346891	0.988750000000000	0.000127600983
(1/500, 1/500)	0.997749460084341	0.997750000000000	0.000054113350
(1/2, 1/10)	0.708165550635041	0.662500000000000	6.448428703442
(1/10, 1/50)	0.933034865745016	0.932500000000000	0.057325376002
(1/10, 1/100)	0.938619470752121	0.938125000000000	0.052680640827
(1/50, 1/100)	0.983128381097547	0.983125000000000	0.000343912109
(1/10, 1/500)	0.943094393391416	0.942625000000000	0.049771623573
(1/100, 1/500)	0.993248719543765	0.993250000000000	0.000128915971

Table 4 The error of curvature-based potential in Eq. (29) between a concave curved surface body and a particle ($n=6$)

$(\tilde{c}_1, \tilde{c}_2)$	$(\tilde{U}_{12})_{numerical}$	$(\tilde{U}_{12})_{polynomial}$	$\delta(\times 100\%)$
(1/2, 0)	1.241840400976359	1.281250000000000	3.173483403557
(1/10, 0)	1.055786435796063	1.056250000000000	0.043907005074
(1/50, 0)	1.011248185952910	1.011250000000000	0.000179386931
(1/100, 0)	1.005627066258407	1.005625000000000	0.000205469649
(1/2, 1/2)	1.447129241557622	1.562500000000000	7.972388030678
(1/10, 1/10)	1.111029494156061	1.112500000000000	0.132355248144
(1/50, 1/50)	1.022489957297669	1.022500000000000	0.000982181025
(1/100, 1/100)	1.011251261653109	1.011250000000000	0.000124761585
(1/500, 1/500)	1.002250539915659	1.002250000000000	0.000053870328
(1/2, 1/10)	1.291834449364959	1.337500000000000	3.534938293177
(1/10, 1/50)	1.066965134254984	1.067500000000000	0.050129636653
(1/10, 1/100)	1.061380529247879	1.061875000000000	0.046587509240
(1/50, 1/100)	1.016871618902453	1.016875000000000	0.000332499943
(1/10, 1/500)	1.056905606608584	1.057375000000000	0.044412044792
(1/100, 1/500)	1.006751280456234	1.006750000000000	0.000127186948

5.2 Accuracy of curvature-based potential in Eq. (29)

In the previous section, if $\tilde{k}_n$ is expanded to the second order, we get the curvature-based potential in Eq. (29), which does not include the Gaussian curvature and the form is simplified. We will test the accuracy of Eq. (29) in this section. Firstly, both sides of Eq. (29) are divided by $\tilde{U}_n$ to get the dimensionless form:

$$\left(\tilde{U}_n\right)_{polynomial} = \frac{U_n}{\tilde{U}_n} = 1 + \frac{n-3}{n-4} \left(\lambda \tilde{H}\right) \quad (34)$$

Calculation results are listed in Tables 3 and 4. Although the Gaussian curvature is not included, the accuracy of Eq. (29) is still satisfactory when $\tilde{c}_1, \tilde{c}_2$ are small quantities.

6 Discussion

6.1 Local properties of the curvature-based potential

The integrand in Eq. (19) is:

$$U_n = \frac{C\rho}{\tau^{n-3}} \int_1^\infty \int_0^{2\pi} \frac{1}{\tilde{R}^{n-1}} \left(\tilde{R} - \frac{\lambda}{2\tilde{k}_n} + \frac{\lambda}{2\tilde{k}_n} \sqrt{4(\tilde{R}\tilde{k}_n)^2 + 1} \right) d\theta d\tilde{R} \quad (35)$$

The domain of integration is $[1, \infty)$. Thus, the interaction potential between V_0 and the particle P on S_0 reflects the global properties of the system. However, from physical viewpoint,

the short-range pair potential determines that the particle P mainly interacts with the nearest zone in V_0 . In the final curvature-based formulation of potential, there exists the mean curvature and the Gaussian curvature, which represents the local properties of V_0 at point P . Thus, from the mathematical viewpoint, the distribution of integrand $g(\tilde{R}, \tilde{k}_n)$ is of highly local properties. For convex and concave V_0 , there are:

$$\widehat{g}(\tilde{R}, \tilde{k}_n) = \frac{1}{\tilde{R}^{n-1}} \left(\tilde{R} + \frac{1}{2\tilde{k}_n} - \frac{1}{2\tilde{k}_n} \sqrt{4(\tilde{R}\tilde{k}_n)^2 + 1} \right) \quad (36)$$

$$\check{g}(\tilde{R}, \tilde{k}_n) = \frac{1}{\tilde{R}^{n-1}} \left(\tilde{R} - \frac{1}{2\tilde{k}_n} + \frac{1}{2\tilde{k}_n} \sqrt{4(\tilde{R}\tilde{k}_n)^2 + 1} \right) \quad (37)$$

The distribution diagrams of Eqs. (36) and (37) are shown in Fig. 7a and b, respectively. From the diagrams we can see that the values of the integrand mainly

Fig. 7 **a** Distribution of the integrand g for convex V_0 and the particle P when $n=12$, $\tilde{c}_1 = 0.1$, $\tilde{c}_2 = 0.05$. **b** Distribution of the integrand $\check{g}$ for concave V_0 and the particle P when $n=12$, $\tilde{c}_1 = 0.1$, $\tilde{c}_2 = 0.05$

Fig. 8 Relationship of the interaction potential between the particle and the infinite body as well as convex and concave curved surface body

distribute in the region of the dimensionless radius $\tilde{R} \in [1, 2]$. Beyond that region, the integrand decreases to zero rapidly.

In Fig. 7, the choice of two principal curvatures is arbitrary. The highly local properties exist for different $\tilde{c}_1$ and $\tilde{c}_2$ when they are small quantities, and the larger the values of $\tilde{c}_1$ and $\tilde{c}_2$ are, the more local the distribution of the function g is. For a particle located on a curved surface body with the same $\tilde{c}_1$ and $\tilde{c}_2$, values of the integrand mainly distribute in the region of $\tilde{R} \in [1, 4]$. Thus, the local property is more remarkable.

6.2 Interaction potentials between particle and two dually-curved surfaces

As shown in Fig. 8a, a particle P in an infinite body is studied. The potential is:

$$U_n^0 = \frac{4\pi C\rho}{(n-3)\tau^{n-3}} = 2\bar{U}_n \quad (38)$$

Suppose the infinite body is composed of two dually-curved surfaces. One is a convex curved surface and the other is a concave curved surface. The particle P is located on the interface of the two dually-curved surfaces. The interaction potentials between the particle P and two dually-curved surfaces are as follows, respectively:

$$U_n = \bar{U}_n \left[1 + \frac{n-3}{n-4} (\lambda \tilde{H}) - \frac{1}{2} \cdot \frac{n-3}{n-6} (\lambda \tilde{H}) (5\tilde{H}^2 - 3\tilde{K}) \right] \quad \lambda = -1 \quad (39)$$

$$\check{U}_n = \bar{U}_n \left[1 + \frac{n-3}{n-4} (\lambda \tilde{H}) - \frac{1}{2} \cdot \frac{n-3}{n-6} (\lambda \tilde{H}) (5\tilde{H}^2 - 3\tilde{K}) \right] \quad \lambda = +1 \quad (40)$$

The following relationship exists:

$$\hat{U}_n + \check{U}_n = U_n^0 \quad (41)$$

Equation (41) indicates that the summation of the interaction potentials U_n and $\bar{U}_n$ is a constant at any point P on the interface, which means that U_n and $\bar{U}_n$ are dual with each other. From physical diagrams, the existence of duality is inevitable: the duality between two curved-surface bodies in Fig. 8 leads to the duality between the two curvature-based potentials in Eq. (41).

Fig. 9 The tangential driving force of the particle on the surface of a curved surface body

6.3 The driving force acting on the particle

The dimensional form of the curvature-based potential in Eq. (28) is:

$$U_n = \overline{U}_n \left[1 + \frac{n-3}{n-4} (\lambda H) \tau - \frac{1}{2} \cdot \frac{n-3}{n-6} (\lambda H) (5H^2 - 3K) \tau^3 \right] \quad (42)$$

Then the tangential driving force acting on the particle P is shown in Fig. 9:

$$\mathbf{F}_t = -(\nabla U_n) = -\left(\frac{\partial U_n}{\partial H} \nabla H + \frac{\partial U_n}{\partial K} \nabla K \right) \quad (43)$$

Here, $\nabla(\dots)$ is the gradient operator defined in the surface S_0 , which lies in the tangent surface. Substituting Eq. (42) into Eq. (43) may give the detailed formulation of the tangential driving force:

$$\mathbf{F}_t = -\overline{U}_n \lambda \tau \left[\frac{n-3}{n-4} \nabla H - \frac{1}{2} \cdot \frac{n-3}{n-6} (15H^2 \nabla H - 3K \nabla H - 3H \nabla K) \tau^2 \right] \quad (44)$$

Equation (44) provides valuable insights in the following respects:

- A highly curved surface will induce a tangential driving force on the particle on the surface. The controlling factors are the mean curvature H , Gaussian curvature K , the gradient of mean curvature ∇H , and the gradient of the Gauss curvature ∇K .
- If the curvature-based potential is taken as Eq. (29), then the tangential force $\mathbf{F}_t$ includes only the first term in Eq. (44), i.e., there only exists the gradient of mean curvature ∇H and the direction of $\mathbf{F}_t$ is only controlled by ∇H .
- Two dually-curved surfaces (with $\lambda = -1$ and $\lambda = +1$, respectively) will act opposite to the tangential driving forces on a particle located on the interface.
- The directions of tangential driving forces acted by convex and concave curved surfaces are opposite. This property strongly affects the surface topography of soft materials, since the tangential driving force determines the direction of motion of particles on the surface, and controls the evolution of surface topography.

- (e) For the sphere, $\nabla H = \mathbf{0}$, $\nabla K = \mathbf{0}$, $\mathbf{F}_t = \mathbf{0}$. Thus the tangential driving force is zero, and the particle can maintain equilibrium on the sphere.
- (f) For the cylinder, $\nabla H = \mathbf{0}$, $\nabla K = \mathbf{0}$, $\mathbf{F}_t = \mathbf{0}$. Thus, the particle on the surface of a cylinder can also maintain balance.
- (g) For a minimal surface, $H = 0$, $\mathbf{F}_t = \mathbf{0}$. Particles on the minimal surface also feel no tangential force and may maintain equilibrium.

The above analysis may explain why spheres, cylinders, and minimal surfaces so widely exist in soft materials.

Recently, many experiments on electro-wetting on curved surfaces have been done by the group of Zhao [17]. They found that the variation of the contact angle is curvature-dependent, and with a decrease of the system size, the surface curvature effect is more significant. Comparing with the planar situation, the contact angle variation decreases on convex surfaces but increases on concave surfaces. These phenomena can be explained from the view of curvature-based potential and curvature-based driving force. Actually, the contact angle is controlled by the interaction potential between a curved substrate and liquid. From Eq. (29), the interaction potential of a curved body and a particle is a function of the interaction potential between a flat body and a particle modified with curvatures. The greater the curved body is, the larger the effect of the curvature is. For concave and convex curved surface bodies, the effect of curvatures is just the opposite. The interaction potential between a concave body and a particle is smaller than the one of a flat body and a particle, while the interaction potential between a convex body and a particle is larger than that of a flat body and a particle. Changing the bending direction of steric configuration will reflect on the sign of curvatures. Curvatures are crucial elements to describe and study micro/nano abnormal phenomena.

6.4 Objectivity of curvature-based potential

Note that all the formulations above are established on the assumption that the positive direction of the z -axis points to the concave side of the outer surface S of V . However, researchers are of course free to choose a positive direction for the z -axis. The potential we study will not change regardless of the positive direction of the z -axis we choose. In other words, the interaction potential of the particle and body must be kept the same. It will not be changed by observers, a property which is called the objectivity of the curvature-based potential.

In the above curvature-based potential, there are odd terms of mean curvature H , which change sign along with the change of the positive direction of the z -axis. In Eq. (28), H is accompanied by the symbol λ . Thus, when the positive direction of the z -axis changes, the sign of the symbol λ must change at the same time, which assures the curvature-based potential to be independent of the positive direction of the z -axis.

When the positive direction of the z -axis points to the concave side of the outer surface S , λ is defined as in Eq. (15). Then, when the positive direction of the z -axis points to the convex side of the outer surface S , the sign of λ should be defined as follows:

$$\lambda = \begin{cases} +1 & \text{for convex curved surface} \\ -1 & \text{for concave curved surface} \end{cases} \quad (45)$$

Thus, although the sign of H and λ changes along with the positive direction of the z -axis, the sign of λH remains the same. Thus, the objectivity of curvature-based potential is guaranteed.

7 Conclusions

At micro/nano scales, for a particle located on the surface of curved surface body, the interaction potential between them can be written as a function of curvatures, which confirms the previous propositions further: a highly curved surface body will induce a driving force, and curvatures and the gradient of curvatures are the essential elements forming the driving forces. For particles on the surface of a curved surface body, tangential driving forces acting on them are of essential importance for understanding the movements of soft materials at micro/nano scales.

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