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Surface integration approach: A new technique for evaluating geometry dependent forces between objects of various geometry and a plate

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ABSTRACT

We present a new approach, which can be considered as a generalization of the Derjaguin approximation, that provides exact means to determine the force acting between a three-dimensional body of any shape and a half-space mutually interacting via pairwise potentials. Using it, in the cases of the Lennard-Jones, standard and the retarded (Casimir) van der Waals interactions we derive exact expressions for the forces between a half-space or a slab of finite thickness and an ellipsoid in a general orientation, which in the simplest case reduces to a sphere, a tilted fully elliptic torus, and a body obtained via rotation of a single loop generalized Cassini oval, a particular example of which mimics the shape of a red blood cell. The results are obtained for the case when the object is separated from the plane via a non-polar continuous medium that can be gas, liquid or vacuum. Specific examples of biological objects of various shapes interacting with a plate like substrates are also considered.

1. Introduction

The Derjaguin approximation (DA) [1,2] allows to determine the forces between two gently curved colloidal particles in a close proximity, or a particle and a half-space bounded by a smooth plane surface, based on the knowledge of this interaction between two planar half-spaces which is normally much easier to be determined analytically. Further, we are going to use the term *plate* instead of *half-space bounded by a smooth plane surface* for simplicity. More specifically, the DA states that the interaction force $F^{R_1,R_2}(L)$ between two curved surfaces with curvatures R_1 and R_2, separated by a distance L is:

$$F^{R_1,R_2}(L) = 2\pi R_{\text{eff}} \int_L^\infty F_A^{\parallel}(z)dz = 2\pi R_{\text{eff}}\, \varphi_A^{\parallel}(L), \tag{1}$$

where $R_{\text{eff}}^{-1} = R_1^{-1} + R_2^{-1}$ is the effective radius, $F_A^{\parallel}$ – the force per unit area between plates, and $\varphi_A^{\parallel}$ is the corresponding potential of interaction per unit area of the plates. As it is clear from the above expression the DA assumes that the force on an infinitesimally small area of one curved surface is due to the interaction with locally flat portions on the other curved surface which implies R_1, $R_2 \gg L$. When the sphere with radius $R_1 \equiv R$ interacts with a flat surface one has $R_2 = \infty$ and then Eq. (1) is still valid with $R_{\text{eff}} = R$, i.e.:

$$F^{R,|}(L) = 2\pi R \varphi_A^{\parallel}(L). \tag{2}$$

Let us note that despite being called, in some areas, proximity "theorem" the DA is simply an approximation and is not valid in a strictly mathematical sense. It is normally assumed that the DA would appear to be justified as long as the colloids are larger than the range of the intermolecular interactions. As it is clear from the above the DA is particularly useful in generalizing theoretical results for planar geometries and is often explicitly (or implicitly) used when interpreting measurements with the surface force apparatus (SFA) [3]. It is important to note that despite of its limitations the DA is widely used for calculations of the interaction potential/force between colloidal particles of various geometries – see, e.g., and the literature cited therein [4–10].

In the current article we will propose a generalization of the DA that allows to determine the *exact* interaction between a three-dimensional (3d) body of any shape with a plate provided that they both are immersed in a non-polar continuous medium that can be gas, liquid or vacuum, and the interaction can be considered as due to pairwise potentials. Concrete examples for specific bodies will be presented for the cases of Lennard-Jones, standard and the retarded (Casimir) van der Waals interactions and some concrete examples concerning the application of the approach proposed for studying biological objects will be discussed. We will term

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our approach a “surface integration approach” (SIA) to be described in the next section.

The structure of the article is as follows. In Section 2 we introduce and derive the general expressions of the SIA technique. In Section 3 we derive closed-form analytical expressions for the interaction of objects of specific geometric shape with a plate or slab of finite thickness. We consider the cases of the interaction of solid sphere with a half-space – Section 3.1, spherical shell and a slab of finite thickness – Section 3.2, arbitrarily orientated solid ellipsoid and a half-space – Section 3.3, arbitrarily orientated ellipsoidal shell and a slab of finite thickness – Section 3.4, tilted fully elliptic torus and a half-space – Section 3.5, a solid body obtained via rotation of a single loop generalized Cassini oval and a half-space – Section 3.6, a shell obtained via rotation of a single loop generalized Cassini oval and a slab of finite thickness – Section 3.7. We study the cases of interactions represented via pair-wise standard and retarded (Casimir) van der Waals interaction and Lennard-Jones potential. Application of the analytical results derived for the evaluation of the interaction of biological objects with a planar substrate (phospholipid bilayer) are presented in Section 4. The article closes with a “Discussion and concluding remarks” section. The technical details needed to obtain the analytical results for the tilted fully elliptic torus are given in Appendix A.

2. Surface integration approach

If the continuous medium (gas, liquid or vacuum) between a body of some general shape and a plate are in a thermodynamic equilibrium the pressure $p(\mathbf{r})$ at any point $\mathbf{r}$ on the surface of the body immersed in this medium will be along the normal $\mathbf{n_r}$ to its surface at that point. Then, integrating over the closed surface S of the object, one obtains the force $\mathbf{F}$ acting on such an object

$$\mathbf{F} = \oint_S p(\mathbf{r})\mathbf{n_r}\, dS. \tag{3}$$

In the case of a force $\mathbf{F}^{R,|}(L)$ between a sphere of radius R and a plate at closest distance L from the sphere for the projection $F^{R,|}(L)$ of the force on the normal from the center of the sphere to the plate, taken to be the z-axis, one obtains

$$F^{R,|}(L) \;\equiv\; \mathbf{F}^{R,|}(L)\cdot \mathbf{e}_z = 2\pi R \int_L^{L+2R} \left[1 - \frac{z-L}{R}\right] F_A^{\|}(z)dz, \tag{4}$$

(see below for more details), where $\mathbf{e}_z$ is a unit vector pointing along the z axis from the sphere to the plate. The above is the simplest example of what we will call the “surface integration approach” (SIA) for the calculation of the force acting between a body and a plate. Under the assumptions for which Eq. (3) is valid the above result for the sphere-plate force is exact and it obviously reduces to the DA, see Eq. (2), if one takes the limit $R \to \infty$ in the integral in Eq. (4). For a material body B (say, colloidal particle), $B \equiv \{(x, y, z), (x, y, z) \in B\}$, of a general shape $S(x, y) = z$ interacting with a (x, y)-plane the corresponding result, see the derivation below, is

$$F^{B,|}(L) = \int_{A_S}\int F_A^{\|}[S(x,y)] \frac{\mathbf{n}_{S(x,y),x,y}\cdot \mathbf{e}_{S(x,y)}}{|\mathbf{n}_{S(x,y),x,y}\cdot \mathbf{e}_{S(x,y)}|}dx\,dy, \tag{5}$$

where A_S is the projection of the surface S of the particle, defined as $S(x, y) = z$, over the plate it interacts with. In Eq. (5) the projection plane is taken to coincide with the (x, y)-plane of the coordinate frame. Note that Eq. (5) has a very simple intuitive meaning: in determining the force acting on the particle one has to subtract from the contributions stemming from surface regions that “face towards” the projection plane those from regions that “face away” from it. Denoting the projections of the corresponding parts of the surface of the body on the (x, y)-plane as $A_S^{\rm to}$ and $A_S^{\rm away}$, where $A_S = A_S^{\rm to} \bigcup A_S^{\rm away}$, Eq. (5) can be simplified to

$$F^{B,|}(L) = \int_{A_S^{\rm to}}\int F_A^{\|}[S(x,y)]dx\,dy - \int_{A_S^{\rm away}}\int F_A^{\|}[S(x,y)]dx\,dy. \tag{6}$$

In the simplest case of a sphere, considered in Eq. (4), the above implies that the contributions will be of the same sign as $F_A^{\|}(z)$ for $z < L + R$, and of opposite sign for $z > L + R$.

Expression Eq. (6) provides means to determine the *exact* interaction of a material body of *any* shape with a planar surface from the *only* knowledge of the plate–plate interactions. In that respect it represents a valuable generalization of the original Derjaguin approximation.

Let us now briefly demonstrate the validity of Eqs. (4)–(6) for any material body in front of a planar surface for any interaction that allows a representation in terms of point-like sources.

Let $\varphi^{p,|}(L)$ is the potential of interaction of a point-like object at a distance L in front of a plate bounded by the (x, y)-plane of the coordinate frame. Then, let $\varphi_A^{\|}(L)$ is the corresponding potential of interaction, per unit area, between two plates a distance L apart along the z-axis. Obviously

$$\varphi_A^{\|}(L) = \int_L^{\infty} \varphi^{p,|}(z)dz, \tag{7}$$

provided that $\lim_{L\to\infty}\varphi_A^{\|}(L) = 0$, which is normally the case for any reasonably fast decaying potential of interaction. Let V is the volume of a body B in front of a plate at distance L of closest approach to it. For the potential $\varphi^{B,|}(L)$ of interaction of B with the plate one obtains

$$\varphi^{B,|}(L) = \int_V \varphi^{p,|}(z)dx\,dy\,dz = \int_L^{L+D} A(z-L)\varphi^{p,|}(z)dz = \int_L^{L+D} F_A^{\|}(z)A(z-L)dz. \tag{8}$$

In Eq. (8) $A(z)$ is the area of the cross section of the body with a plane parallel to the (x, y)-plane at distance z from it. There D is the length of the orthogonal projection of B on the z-axis. In the last line of Eq. (8) we have used Eq. (7) and the relation

$$F_A^{\|}(L) = -\frac{d}{dL}\varphi_A^{\|}(L). \tag{9}$$

Now, on the basis of Eq. (8) and the fact that

$$F^{B,|}(L) = -\frac{d}{dL}\varphi^{B,|}(L), \tag{10}$$

one obtains that:

$$F^{B,|}(L) = F_A^{\|}(L)A(0) - F_A^{\|}(L+D)A(D) + \int_L^{L+D} F_A^{\|}(z)\frac{d}{dz}A(z-L)dz. \tag{11}$$

Performing an integration by parts in the last term of Eq. (11) one derives

$$F^{B,|}(L) = -\int_L^{L+D} A(z-L)\left(\frac{d}{dz}F_A^{\|}(z)\right)dz = -\int_V \frac{d}{dz}F_A^{\|}(z)dx\,dy\,dz = \int_V {\rm div}\left(F_A^{\|}\mathbf{e}_z\right)dV = \oint_S F_A^{\|}\mathbf{e}_z\cdot d\mathbf{S}, \tag{12}$$

or, in other words

$$\mathbf{F}^{B,|}(L)\cdot \mathbf{e}_z = \oint_S F_A^{\|}\mathbf{e}_z\cdot d\mathbf{S}. \tag{13}$$

Since the x and y components of $\mathbf{F}^{B,|}(L)$ under the symmetry given in the problem are zero, one can generalize Eq. (13) into

$$\mathbf{F}^{B,|}(L) = \oint_S F_A^{\|}d\mathbf{S} = \oint_S F_A^{\|}\mathbf{n_r}\, dS, \tag{14}$$

which is the statement analogous to Eq. (3). From Eq. (14) it is straightforward to derive Eq. (5) and, as a particular case, Eq. (4).