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Approximate expression of Young's equation and molecular dynamics simulation for its applicability*

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In 1805, Thomas Young was the first to propose an equation (Young's equation) to predict the value of the equilibrium contact angle of a liquid on a solid. On the basis of our predecessors, we further clarify that the contact angle in Young's equation refers to the super-nano contact angle. Whether the equation is applicable to nanoscale systems remains an open question. Zhu *et al.* [*College Phys.* **4** 7 (1985)] obtained the most simple and convenient approximate formula, known as the Zhu–Qian approximate formula of Young's equation. Here, using molecular dynamics simulation, we test its applicability for nanodrops. Molecular dynamics simulations are performed on argon liquid cylinders placed on a solid surface under a temperature of 90 K, using Lennard–Jones potentials for the interaction between liquid molecules and between a liquid molecule and a solid molecule with the variable coefficient of strength a. Eight values of a between 0.650 and 0.825 are used. By comparison of the super-nano contact angles obtained from molecular dynamics simulation and the Zhu–Qian approximate formula of Young's equation, we find that it is qualitatively applicable for nanoscale systems.

Keywords: molecular dynamics simulation, Young's equation, surface tension, Zhu–Qian approximate formula of Young's equation

PACS: 68.08.Bc, 68.03.Cd, 61.46.Fg, 87.10.Tf **DOI:** 10.1088/1674-1056/28/1/016801

1. Introduction

With the rapid development of nanotechnology in recent years, the nanoscale capillarity theory has become a very important research branch. It has a profound influence on surface science, fluid dynamics, micro-electro-mechanical systems, bioscience, and some application areas. The formula to determine the contact angle based on thermodynamic theory of capillary phenomena is Young's equation[1]

$$\cos\theta = \frac{\gamma_{sv} - \gamma_{sl}}{\gamma_{lv}}, \tag{1}$$

where γ_{lv}, γ_{sl}, and γ_{sv} are the liquid–vapor, solid–liquid, and solid–vapor interfacial tensions, respectively, and θ is the equilibrium contact angle measured through the liquid (see Fig. 1).

If the contact angle is smaller than 90°, the solid surface is said to be wetted (hydrophilic), and if the contact angle is larger than 90°, the solid surface is said to be non-wetted (hydrophobic). It is obvious that Young's equation does not consider the influence of the tension of the three-phase contact line on the contact angle, so it is only applicable to the case where the tension of the three-phase contact line is negligible, such as the solid–liquid contact of the cylindrical liquid whose axis of symmetry is parallel to the solid plane.

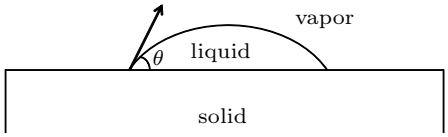


Fig. 1. Schematic of a liquid drop on a solid surface showing the contact angle: $\theta < 90°$ wetting, and $\theta > 90°$ non-wetting.

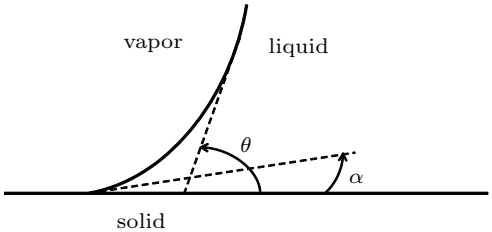


Fig. 2. Schematic figure of super-nano contact angle and nano contact angle.

In 1976, Jameson *et al.*[2] noticed that Young's equation might not describe the actual contact angle. In 1977, White[3] argued that Young's equation did not concern itself with the microscopic contact angle (nano contact angle α in our paper),

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but it could really determine the macroscopic contact angle θ that the vapor–liquid interface makes with the solid–liquid interface at microscopically large distances from the contact line, as shown in Fig. 2. However, this microscopically large distance does not need to reach the real macroscopic distance, so this contact angle is more accurately called the super-nano contact angle θ in the present paper.

Although thermodynamically sound,[4,5] Young's equation cannot be verified experimentally, since the surface tensions of solids can only be inferred and cannot be directly measured. Now the contact angle is being used to characterize the interactions of liquids with solids of near-molecular dimensions, such as carbon nanotubes[6] and nanocones.[7] In these experiments, Young's equation is used on trust, with limited detailed evidence of its applicability for these small systems.[8] Its applicability to the nanoscale systems remains an open question.[9,10] Therefore, it has attracted many theoretical and experimental studies, where most of the theoretical studies are based on molecular dynamics simulation.[11–16] Sikkenk *et al.*[11] carried out molecular dynamics simulations of Lennard–Jones atoms in a rectangular box and used Young's equation to calculate the super-nano contact angle at the triple point temperature. They found a large deviation between the measured values and the values predicted by Young's equation. Among the studies devoted to these problems, the studies by Nijmeijer and coworkers[12] are one of the most important references since the theoretical formula of solid–fluid surface tensions was obtained for different solid interfaces: smooth plane or atom periodic arrangement of a crystal superficial plane. These studies also explored the physical properties of interfaces by simulating the model systems of particles under Lennard–Jones pair interaction potential. They replaced the live wall with an inert wall and concluded that there were agreements with Young's equation for non-wetting, but had large error for wetting. In 2002, Maruyama *et al.*[13,14] also simulated the super-nano contact angle of argon liquid on a virtual solid wall. They calculated various super-nano contact angles by changing the parameter in the potential between argon and the virtual solid wall. They concluded that the super-nano contact angle decreases with the increase of the interface potential. This does not seem to contradict the Young's equation except the quantitative relationship. Recently, Seveno *et al.*[15] investigated Young's equation through molecular dynamics simulations of a cylindrical rod dipping into a liquid bath. They found very good agreement between the measured force and that predicted by Young's equation. However, several recent articles have already questioned the validity of Young's equation at this small scale.[17,18]

On the other hand, some researchers have proposed the density functional theory approach and molecular dynamics approach to determine the nano contact angle.[19–23] We reviewed and commented the approaches,[19] and improved the simplified approximate form for the molecular dynamics theory of nano contact angle given by Zhu in 1995. A simple improved formula for nano contact angle with two optimum parameters x and k is obtained. Despite all this, the super nano contact angle plays an important role in determining the shape of nanoscale systems; therefore, it is still necessary to use molecular dynamics methods to study its accuracy, i.e. error.

In Young's equation (Eq. (1)), θ and $\gamma_{\rm lv}$ can be experimentally measured. Because the molecules of solids cannot move more freely than those of liquids and vapors, it is difficult to measure $\gamma_{\rm sv}$ and $\gamma_{\rm sl}$. The work is very heavy for using the molecular dynamics approach to calculate $\gamma_{\rm sv}$ and $\gamma_{\rm sl}$ independently with sufficient precision. In order to explore the applicability of Young's equation, researchers often use equivalent or approximate formulas to easily solve and calculate surface tension or super-nano contact angle.

Simplifying the intermolecular force into an attractive hard sphere model and ignoring the temperature effect, Zhu *et al.*[24] derived the approximately equivalent form of Young's equation in 1985. Our work is devoted to studying the applicability of the Zhu–Qian approximate Young's equation for more general situations. Molecular dynamics simulations are carried out on argon liquid cylinders placed on a solid surface under a temperature of 90 K, using Lennard–Jones potentials for the interaction between liquid molecules and between a liquid molecule and a solid molecule with the variable coefficient of strength a. Eight values of a between 0.650 and 0.825 are used. Comparing the super-nano contact angles obtained from molecular dynamics simulation and Zhu–Qian approximate Young's equation, we find that the Zhu–Qian approximate Young's equation is qualitatively applicable.

The rest of the present paper is organized as follows. In Section 2, we introduce the Zhu–Qian approximate formula of Young's equation. In Section 3, we describe the molecular dynamics simulation, results, and discussion. The conclusion is given in Section 4.

2. Zhu–Qian approximate formula of Young's equation

Simplifying the intermolecular force into an attractive hard sphere model and ignoring the temperature effect, Zhu *et al.*[24,25] once obtained an approximate formula of Young's equation. They proposed the concepts of weighted average effective adhesive force and weighted average effective cohesive force. Then they deduced the expression of the super-nano contact angle through the principle of minimum potential energy

$$\cos\theta = (2\overline{f}^a_{\rm sl} - \overline{f}^a_{\rm ll})/\overline{f}^a_{\rm ll}, \tag{2}$$

where $\overline{f}^a_{\rm ll}$ is the weighted average effective cohesive force

$$\overline{f}^a_{\rm ll} = \int_0^e \xi f_{\rm ll}(\xi){\rm d}\xi \Big/ \int_0^e \xi {\rm d}\xi, \tag{3}$$

and $\overline{f}^a_{\rm sl}$ is the weighted average effective adhesive force

$$\overline{f}^a_{\rm sl} = \int_0^e \xi f_{\rm sl}(\xi){\rm d}\xi \Big/ \int_0^e \xi {\rm d}\xi. \tag{4}$$

Here, e is the thickness of the adhesive layer, ξ is the distance from the liquid molecule to the liquid–vapor interface, $f_{\rm ll}(\xi)$ is the interaction force of liquid atoms in the internal liquid, and $f_{\rm sl}(\xi)$ is the interaction force between liquid atoms and the solid on which they are located. Equation (2) is the Zhu–Qian approximate Young's equation, and it gives the wetting condition: the solid surface is considered to be wetted (hydrophilic) if $\overline{f}^a_{\rm sl} > \overline{f}^a_{\rm ll}/2$, the solid surface is considered to be non-wetted (hydrophobic) if $\overline{f}^a_{\rm sl} < \overline{f}^a_{\rm ll}/2$.

Let $U_{\rm ll}(r)$ be the interaction potential energy between liquid molecules, and $U_{\rm sl}(r)$ be the interaction potential energy between a liquid molecule and solid molecule. For cases where $f_{\rm ll}(\xi)/f_{\rm sl}(\xi)$ is not related to ξ, we have

$$f_{\rm ll}(\xi)/f_{\rm sl}(\xi) = \overline{f}_{\rm sl}/\overline{f}_{\rm ll} = U_{\rm sl}(r)/U_{\rm ll}(r) = a, \tag{5}$$

where a is the relative coefficient of strength. By substituting this condition into Eq. (2), we obtain another Zhu–Qian approximate formula of Young's equation

$$\cos\theta = 2a - 1. \tag{6}$$

We can see that equation (6) is simple and easy to verify.

3. Molecular dynamics simulation, results, and discussion

3.1. Molecular dynamics simulation

We adopt cylindrical liquid–vapor equilibrium systems placed on a solid surface to analyze and simulate the acceptable statistics under a periodic boundary condition. In this case, the three-phase contact line is a straight line, and the line tension does not affect the contact angle, which is consistent with Young's equation and its approximate equation.

As the initial configuration, argon liquid semi-cylinders are placed on the solid surface, consisting of 13800 argon atoms. The central axis is in the x direction. A simple cubic structure of a solid with three layers is placed at the bottom of the calculation cell (z=0, $-\sigma$, -2σ), consisting of 8154 solid atoms. The rest of the solid is treated as a continuum model ($z \leqslant -3\sigma$). The box size of the simulation system is $0 \leqslant x \leqslant 18\sigma$, $-75\sigma \leqslant y \leqslant 75\sigma$, and $0 < z < 45\sigma$. The periodic boundary condition is used in the x direction and the mirror boundary condition is used in the y and z directions.

In molecular dynamics simulations, the intermolecular interactions between argon atoms are described by the Lennard–Jones potential

$$U_{\rm ll}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right], \tag{7}$$

where r, ε, and σ are the interparticle distance, energy scale, and length scale, respectively. We adopt the Lennard–Jones potentials for the interaction between liquid molecules and between a liquid molecule and a solid molecule with the variable coefficient of strength a, which has been used in Eq. (5)

$$U_{\rm sl}(r) = 4a\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]. \tag{8}$$

In our simulations, eight values of a between 0.650 and 0.825 are used. The interactions between argon atoms and solid atoms are discussed in two cases: the interactions between argon atoms and the first three layers of solid atoms are given by Lennard–Jones potential with the cut-off distance 3σ, and the interactions between argon atoms and the rest of the solid atoms are given by Eq. (9) instead of Eq. (8)

$$E = -\pi n a \varepsilon \sigma^6/(6(\Delta z)^3), \tag{9}$$

where n is the atom number density, and we choose n=1/σ^3 in the molecular dynamics simulation; Δz is the distance between argon atoms and the fourth-layer atoms of the solid.[26]

All quantities used in the simulation are dimensionless. According to the basic parameters of an argon atom, m = 6.3382 $\times 10^{-26}$ kg, $\varepsilon = k_{\rm B}120$ K ($k_{\rm B}$ = 1.38 $\times 10^{-23}$ J/K), and σ = 0.3405 nm, and the dimensionless quantities are as follows: $r^* = r/\sigma$ for length, $T^* = k_{\rm B}T/\varepsilon$ for temperature, $t^* = t\sqrt{(\varepsilon/m\sigma^2)}$ for time, $\rho^* = \rho\sigma^3/m$ for density, $f^* = f\sigma/\varepsilon$ for force, and $E^* = E/\varepsilon$ for energy. The simulated temperature is $T^* = 0.75$. The cut-off distance is $r_{\rm c} = 3.0$.

For the cylindrical liquid systems, at the initial time, the velocities of all the particles are given according to the Maxwell–Boltzmann distribution. The velocity–Verlet algorithm[27] is used in molecular dynamics. The canonical ensemble of temperature 90 K and time step $\delta t = 5$ fs is used before equilibrium. On calculating the mean value of a physical quantity, we change the time step to $\delta t = 2$ fs. In order to find the step number N that is needed for a physical quantity $g(t)$ to reach its steady value, we use an accumulative average method for the statistics

$$\overline{g(i\cdot\delta t)}^N = \frac{1}{N}\sum_{i=1}^{N} g(i\cdot\delta t), \tag{10}$$

where the number $\overline{g(i\cdot\delta t)}^N$ must be large enough for the accumulative mean value to reach a constant with acceptably small variation. In fact, 10^6 runs with a time step of $\delta t = 2$ fs were used to obtain acceptable statistics in our simulations. A snapshot of the simulated system with N = 13800 and a = 0.750 after equilibrium is shown in Fig. 3.

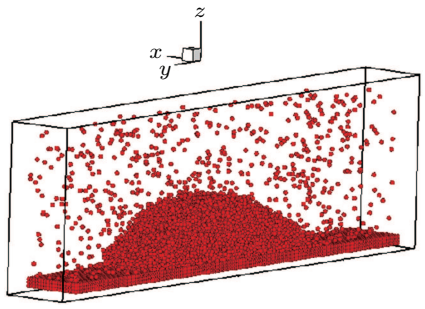


Fig. 3. A snapshot of the simulated system with variable coefficient of strength $a = 0.750$ after equilibrium.

3.2. Results and discussion

Figure 4 displays the profile of a cross-section in isodensity space of the argon cylindrical droplet on a solid surface with the coefficient of strength $a = 0.750$. They are closed curves. The position of solid atoms in the top layer is $z = 0$ in Fig. 4. Because gravity is neglected, the isodensity space is a part of a coaxial cylinder. The radius of the Gibbsian surface of tension and the value of the corresponding height $z = z_0 = 18.31$ are calculated according to Eq. (25) in Ref. [19] (see Ref. [19] for details). The top of the coaxial cylindrical surface tangent to the horizontal line (see Fig. 4) is the intersecting line of the Gibbsian surface of tension. We define the Gibbsian surface of tension as the closed isodensity surface, which is shown in Fig. 5.

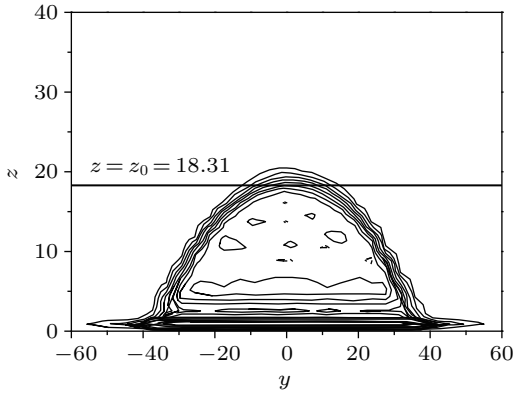


Fig. 4. The profile of the cross-section in isodensity space.

Because we consider argon cylindrical liquid in the simulation, the upper part of the liquid should be a section of a cylinder, and its Gibbsian surface of tension is theoretically a section of part of the cylindrical surface. The upper part of the obtained Gibbsian interface is the Gibbsian surface of tension. The Gibbsian surface of tension above the adhesive layer is fitted as an arc of a circle by using the method of least squares, which is shown in Fig. 6. The super-nano contact angle is defined as the angle between this fitted circle and the horizontal line, where the horizontal line is the boundary between the adhesive layer and the internal liquid.

The values of comparison of the super-nano contact angles of the molecular dynamics simulation and Zhu–Qian approximate formula of Young's equation (Eq. (6)) are listed in Table 1, where θ^* is the measured value from the molecular dynamics simulation, and θ is obtained from the Zhu–Qian approximate formula of Young's equation.

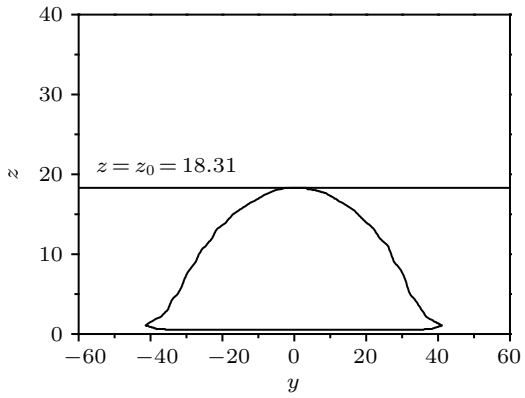


Fig. 5. The shape of the Gibbsian surface of tension.

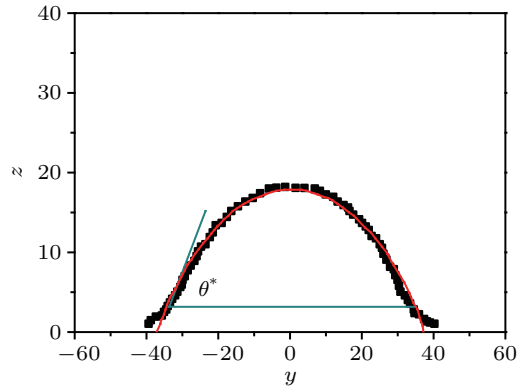


Fig. 6. The fitted shape of the Gibbsian surface of tension.

Table 1. The values of comparison of the super-nano contact angles (°) of the molecular dynamics simulation and Zhu–Qian approximate formula of Young's equation.

a	z_0	θ^*	$\cos\theta^*$	$\cos\theta$	θ	$\Delta\theta$
0.650	22.09	55.50	0.5664	0.30	72.54	17.04.
0.675	20.20	50.78	0.6323	0.35	69.51	18.73.
0.700	19.50	46.40	0.6896	0.40	66.42	20.02
0.725	18.64	43.50	0.7255	0.45	63.26	19.76
0.750	18.31	42.05	0.7426	0.50	60.00	17.95
0.775	17.90	40.60	0.7593	0.55	56.63	16.03
0.800	17.11	37.50	0.7933	0.60	53.13	15.63
0.825	16.38	33.47	0.8417	0.65	49.46	16.00

Figure 7 displays the relation between a and the cosine of θ (θ^*). We can see the $\cos\theta^* - a$ relation is in qualitative agreement with the $\cos\theta - a$ relation, which means the Zhu–Qian approximate formula of Young's equation is qualitatively applicable to the nanoscale systems. The $\cos\theta^* - a$ relation agrees with earlier reports.[28–30] Moreover, since equation (6) is derived via Young's equation, the latter application is qualitatively confirmed at the scale of simulations. However, there is an almost quantitative discrepancy between these two sets of data. Simplifying the intermolecular force into an attractive

hard sphere model and ignoring the temperature effect when deriving Eq. (6) may be the cause of this inconsistency.

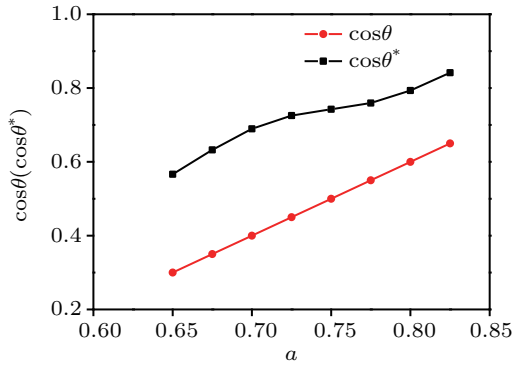


Fig. 7. The relation between a and the cosine of super-nano contact angle.

4. Conclusion

Young's equation now plays a crucial role in nanotechnology, as the super-nano contact angle is being used to characterize the interactions of liquids with solids. Whether the equation is applicable to nanoscale systems remains an open question. Zhu *et al.* obtained the most simple and convenient approximate formula of Young's equation. Using molecular dynamics simulations, we test its applicability to real nanodrops. Molecular dynamics simulations are carried out on argon liquid cylinders placed on a solid surface under a temperature of 90 K, using Lennard–Jones potentials for the interaction between liquid molecules and between a liquid molecule and a solid molecule with the variable coefficient of strength a. Eight values of a between 0.650 and 0.825 are used. By comparing the super-nano contact angles of the molecular dynamics simulation with the Zhu–Qian approximate formula of Young's equation, we find that Young's equation is qualitatively applicable to nanoscale systems. Simplifying the intermolecular force into an attractive hard sphere model and ignoring the temperature effect when deriving the Zhu–Qian approximate formula of Young's equation may be the cause of the result that the Zhu–Qian approximate formula of Young's equation can only be qualitatively established. This remains to be demonstrated. We are currently working toward this end. Our studies will have certain implications for the further use of Young's equation.

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