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Crackling sound generation during the formation of liquid bridges: A lattice gas model

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HIGHLIGHTS

- Expiratory crackle is due to an energy released during the formation of a liquid bridge.
- The magnitude of crackle sound is proportional to the difference in free energy.
- We correlate the force exerted from the liquid bridge with the airway recoil forces.
- Our lattice gas model agrees with analytical calculation based on energy minimization.
- We used our results to study the critical conditions of the liquid bridges formation.

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ABSTRACT

Due to abnormal mechanical instabilities, liquid bridges may form in the small airways blocking airflow. Liquid bridge ruptures during inhalation are the major cause of the crackling adventitious lung sound, which can be heard using a simple stethoscope. Recently, Vyshedskiy and colleagues (2009) [1] described and characterized a crackle sound originated during expiration. However, the mechanism and origin of the expiratory crackle are still controversial. Thus, in this paper, we propose a mechanism for expiratory crackles. We hypothesize that the expiratory crackle sound is a result of the energy released in the form of acoustic waves during the formation of the liquid bridge. The magnitude of the energy released is proportional to the difference in free energy prior and after the bridge formation. We use a lattice gas model to describe the liquid bridge formation between two parallel planes. Specifically, we determine the surface free energy and the conditions of the liquid bridge formation between two parallel planes separated by a distance $2h$ by a liquid droplet of volume Ω and contact angle Θ, using both Monte Carlo simulation of a lattice gas model and variational calculus based on minimization of the surface area with the volume and the contact angle constrained. We numerically and analytically determine the phase diagram of the system as a function of the dimensionless parameter $h\Omega^{-1/3}$ and Θ. We can distinguish two different phases: one droplet and one liquid bridge. We observe a hysteresis curve for the energy changes between these two states, and a finite size effect in the bridge formation. We compute the release of free energy during the formation of the liquid bridge and discuss the results in terms of system size. We also calculate the force exerted from liquid bridge on the planes by studying the dependence of the free energy on the separation between the planes $2h$. The simulation results are in agreement with the analytical solution.

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1. Introduction

The lung airways are coated with surfactants and other organic fluids, and the surface force generated at the air–liquid interface plays a major role in breathing mechanics [2–4]. In certain lung diseases, the surface properties of these fluids are changed and liquid bridges may form in small airways, closing them, and consequently impairing gas exchange [5–9]. The stability, the rupture, and formation conditions of the liquid bridge are strongly influenced by surface tensions at the air–liquid interface and the nature of the solid–liquid contact.

During inspiration, liquid bridges that are closing the airways may pop open due to mechanical instabilities [10–12] and emit a discrete sound event called pulmonary crackle, which can easily be heard using a stethoscope. Lung crackle is an important adventitious lung sound for diagnosis of lung diseases [13–18] and has been an interesting problem in physics, since they are caused by formation and rapture of capillary liquid bridges [19–22] which have been studied extensively in other branches of physics. Recently, Vyshedskiy and colleagues [1] systematically examined the relationship between inspiratory and the uncommon expiratory crackles. These observations were quantitatively consistent with stress relaxation quadrupole hypothesis of crackle generation [23], in which crackles are generated either by the opening or closing of the airways. Here, we evaluate a hypothesis that the expiratory crackles are generated by liquid bridge formation during the closing of the airway. Analogously, the inspiratory crackles are produced by the liquid bridge raptures, a problem studied numerically and analytically in Ref. [22]. To study this problem, we modeled the liquid bridge in a simple geometry: the liquid is trapped between two plane surfaces [22].

1.1. Lattice gas model for the liquid bridge

Lattice gas models have been studied to analyze, interpret, and predict experimental results, including such diverse phenomena as atomic force microscopy [24,25], sintering [26,27], cellular motors [28], and lung sounds [22]. We use a simplified 3D lattice gas model that has been developed to explain inspiratory crackle generation during liquid bridge rupture [22] and validate it by an exactly solvable analytical model based on variational principles. In both models, numerical and analytical, the liquid bridges are axially symmetrical between two semi-wet planes, where the base radius R at both planes is not fixed. For this particular geometry, we could distinguish two stable configurations: (i) when the liquid phase forms a bridge between the two planes, we call it a closed state, and (ii) when the liquid phase forms a droplet on the plane, we call it an open state [22].

The lattice gas model includes particles of three types liquid (l), solid (s), and gas (g). A system consists of liquid of total volume Ω, two solid planes separated by distance $2h$, and surrounding gas. The lattice size is $60 \times 60 \times 52$ with 10 000 liquid particles. We simulate the formation of the liquid bridge between the planes and its rupture using the Monte Carlo method with the Metropolis algorithm. There is no exchange between identical particles, and the exchange between gas and liquid particles are performed randomly according to the Kawasaki dynamics and weighted by the Boltzmann factor, while the solid particles are fixed to maintain the geometry of the planes. We can move the planes in the z direction to change their separation $2h$. Each particle has 26 neighbors: $6 + 12 + 8$, with distances 1, $\sqrt{2}$ and $\sqrt{3}$, respectively. To model the liquid–liquid interaction and liquid–solid interaction, we reduce the interaction strength at distances $\sqrt{2}$ and $\sqrt{3}$ with respect to the interaction strength between the nearest neighbors [22]. The contact angle Θ is set by adjusting the solid–liquid interaction. During this process the lattice gas model evaluates several physical properties such as energy, liquid bridge shape, and surface area.

1.2. Analytical solution

We use the analytical solution to validate the lattice gas model of liquid bridge between two parallel planes [22]. All relevant characteristics of the liquid bridge between two parallel planes are found in terms of elliptic integrals, which depend on their contact angle Θ and the bridge neck to base ratio $a = A/R$, where A is the radius of the neck of the bridge and R is the radius of the circle of contact between the bridge and the plane [22].

A single droplet of liquid attached to one of the two planar surfaces will acquire a shape of a spherical segment of radius R_0, with the center at $(x = 0, y = 0, z = \pm[h + R_0 \cos\Theta])$ forming a circular intersection with the plane of the radius $\rho_0 = R_0 \sin\Theta$, where

$$R_0 = \left(\frac{6\Omega}{2\pi(2 - 3\cos\Theta + \cos^3\Theta)}\right)^{1/3}. \tag{1}$$

In this case, the minimal separation of the planes $h_{\min}$ before the formation of the liquid bridge is

$$2h_{\min} = R_0(1 - \cos\Theta). \tag{2}$$

It was shown in Ref. [22] that the liquid bridge of the same volume Ω is stable at this separation and its free energy $\mathcal{F}_b(\Omega, h_{\min})$ is smaller than the free energy of the single droplet $\mathcal{F}_{0,1}(\Omega)$, which is given by

$$\mathcal{F}_{0,1} = \pi\gamma R_0^2\left[2(1 - \cos\Theta) - \sin^2\Theta\cos\Theta\right], \tag{3}$$

and

$$\mathcal{F}_b(a) \equiv 2\pi h_{\min}^2 \frac{2\sigma(a,1) - \cos\Theta}{u(a,1)^2}, \tag{4}$$

where γ is the surface tension, and a is a dimensionless bridge neck radius, which can be determined from the equation

$$\Omega = 2\pi h_{\min}^3 \frac{v(a,1)}{u(a,1)^3}, \tag{5}$$

and $u(a,1)$, $v(a,1)$, and $\sigma(a,1)$ can be expressed in terms of Legendre elliptic integrals $F(\phi,k)$ and $E(\phi,k)$ as

$$\begin{aligned} u(a,r) &= a\tilde{F}(k,\phi_r) + b\tilde{E}(k,\phi_r), \\ \sigma(a,r) &= (b+a)b\tilde{E}(k,\phi_r), \\ v(a,r) &= \left[-\mathcal{R}(a,r) - a^2 b\tilde{F}(k,\phi_r) + b[3ab + 2(a^2+b^2)]\tilde{E}(k,\phi_r)\right]/3, \end{aligned} \tag{6}$$

where

$$\begin{aligned} b &= \left(\frac{1 - a\sin\Theta}{\sin\Theta - a}\right), \\ k &= s\sqrt{b^2 - a^2}/b, \\ \mathcal{R}(a,r) &= r\sqrt{(r^2-a^2)(b^2-r^2)}, \\ \phi_r &= \arcsin\sqrt{(b^2-r^2)/(b^2-a^2)}, \\ \tilde{F}(k,\phi) &= F(k,\pi/2) - F(k,\phi), \\ \tilde{E}(k,\phi) &= E(k,\pi/2) - E(k,\phi). \end{aligned} \tag{7}$$

This suggests that as soon as a droplet touches the opposite plane, it forms a symmetrical bridge. As soon as the bridge forms, it starts to attract the opposite planes with the force

$$F = 2\pi\gamma \frac{h(1 - a\sin\Theta)}{1(1-a^2)u(a,1)}, \tag{8}$$

which is a monotonically decreasing function of h. Thus the formation of the bridge may lead to the collapse of the space between the planes if the external force keeping the planes apart is less than F. The existing bridge loses its stability and breaks if the half distance between the planes becomes greater than

$$h_{\max} = u(a_c,1)\left(\frac{\Omega}{2\pi v(a_c,1)}\right)^{\frac{1}{3}}, \tag{9}$$

where a_c is the critical neck-base ratio $a_c = \tan(\Theta/2)$, for $\Theta > 31°$.

We study the dependence of the energy gap during the liquid bridge formation with contact angle Θ and relate this energy gap to the crackling bursting sound in the lung. We can compute the free energy difference $\Delta\mathcal{F} = \mathcal{F}_b(\Omega, h_{\min}) - \mathcal{F}_{0,1}(\Omega)$ between the energy of the droplet and the bridge, which will give us the energy released during the liquid bridge formation; see Fig. 1.

2. Results and discussion

In order to compare the results of the lattice gas model with the analytical calculations, we introduce a critical distance $2h_c$ between the planes at which a single droplet of total volume Ω forms a bridge. The abrupt decrease in free energy will then disturb the system as a mechanical perturbation, generating a short bursting sound that we associate with an expiratory crackle [1]. We show that in the lattice gas model h_c is uniquely determined by the dimensionless parameter $\eta(\Theta) = h_c\Omega^{-1/3}$ which depends only on the contact angle; see Fig. 2.

Indeed, we found similarities between simulation and analytical results (Fig. 2). However, Fig. 2 shows that the bridge always forms before the minimal $h_{\min}$ position predicted by analytical calculation. In order to explain this, we notice that due to the effect of the temperature, there are always particles of liquid at the surface of both planes and in the bulk, forming the vapor. In a system with a single droplet in one of the planes moving down, there will be a moment in which the droplet gets very close to the second plane; let us say, three sites apart. See Fig. 3. The surface of the droplet has a spontaneous deformation due to exchange between particles at the liquid–gas interface, associated with the surface's free energy change in the amount of a few $k_B T$. Furthermore, the vapor in the gap between the droplet and the opposite plane will generate an instability, attracting more vapor to the gap, starting an avalanche which will lead to the liquid bridge formation, illustrated

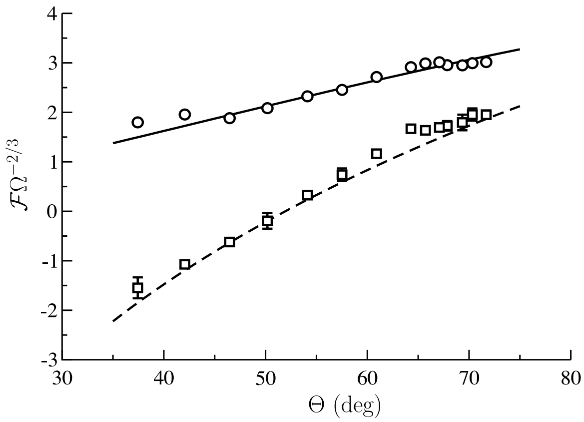

Fig. 1. The normalized free energy $\mathcal{F}\Omega^{-2/3}$ as a function of the contact angle Θ at the moment of the liquid bridge formation with the distance between the planes $2h_{\text{min}}$. The analytical and corresponding numerical maximal free energy of the droplet (continuous line Eq. (3)/open circles) and the liquid bridge (dashed lines Eq. (4)/open squares). The lattice size is $60 \times 60 \times 52$ with 10 000 liquid particles.

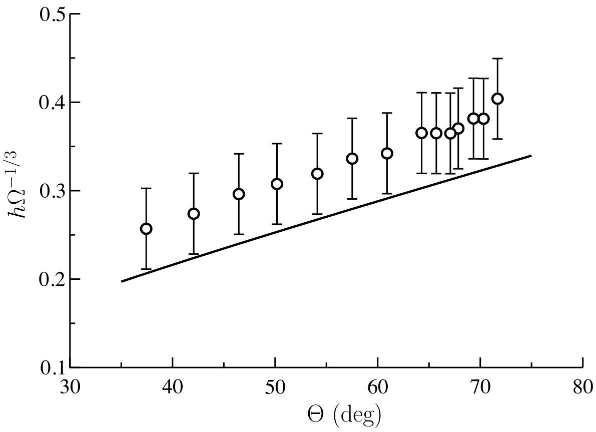

Fig. 2. The minimal half-distance between the two planes h_{min}, for which the droplet is stable, computed using Eq. (2) (solid line) [22]. Circles indicate the value of h_c for which the bridge forms during the numerical simulation. The vertical error bars correspond to 1 lattice cell resolution for the distance in which the rupture is observed. The lattice size is $60 \times 60 \times 52$ with 10 000 liquid particle.

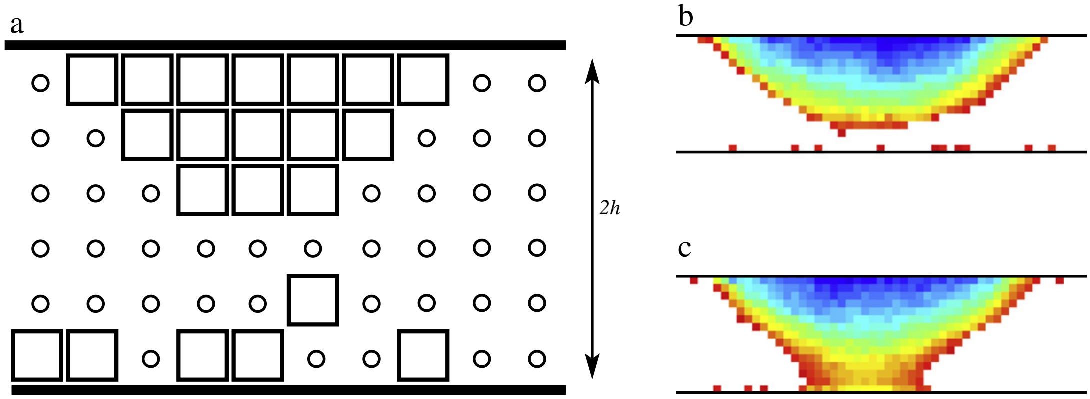

Fig. 3. The illustration of the system near the liquid bridge formation, showing (a) liquid particles (squares), air (circles) and the planes (thick lines). We call vapor the unconnected liquid particles. The liquid particles on the planes are wetting them, and all the remaining liquid particles form the droplet.

in Fig. 3. The vapor effect is very strong and most of the bridges will be formed at this point, which explains the difference in results from the analytical calculation and the lattice gas model. We must highlight that the vapor effect we describe here is not numerical diffusion. In our simulation the exchange dynamics is not limited to neighboring sites; it can happen between any two sites of the lattice. However, we tested the model only allowing particle exchanges within neighboring

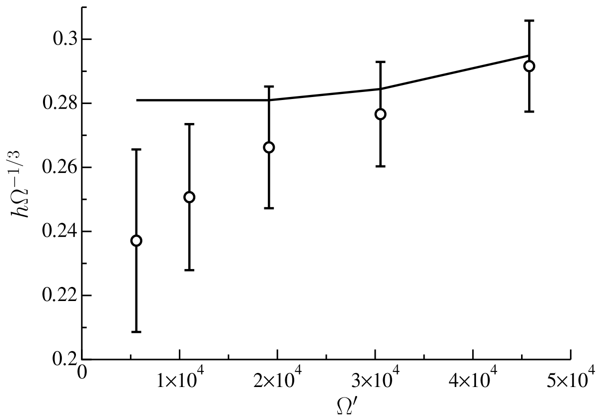

Fig. 4. The system size analysis of the liquid bridge formation for $\Theta \approx 60°$. We study five system sizes keeping the shape of a box and the ratio between liquid and gas particles at the same proportion. The edges of the cubic boxes are 40, 50, 60, 70 and 80, and the corresponding total volume of liquid particles in the system Ω' are 5574, 11 000, 19 140, 30 544, and 45 760. The continuous thick line is the analytical liquid bridge formation distance $h_{\min}$.

ranges and the vapor effect were still present. Indeed, there are always some particles attached to the plane and some particles protruding from the droplet by one site. Hence the particle inserted in between the droplet and the plane may attract to both the droplet and the plane and hence has a larger chance to stay there than in the open space far away from the liquid and plane. Successful insertion of such a particle may lead to an avalanche of insertions into the nearby sites which rapidly fills the gap between the droplet and the wall. Thus, the liquid bridge always forms before the droplet touches the plane. Because of this, we found a small difference between numerical and analytical solutions. The analytical model does not have this effect, because it completely neglects the vapor, and the liquid interface roughness. Thus, the vapor effect cannot be predicted in the analytical calculation, but it can be observed in our model and experimentally in the atomic force microscopy [29].

We can notice that the contact angle Θ does not change much in different system sizes. Next we study the effect of the system size on the bridge formation; see Fig. 4. Thus, we fixed all the interaction parameters $s_{i,j}$ at the value that generates a contact angle of approximately 60°, and then vary the system size. As we increase the system sizes, we also increase the amount of liquid particles, Ω', always keeping constant the air/liquid fraction in the system. For each system size in the numerical model, we calculate the exact value of Θ and found the critical value where the liquid bridge is formed, numerically, h_c, and the analytical constraint $h_{\min}$. Due to the vapor effect, the liquid bridge will always form two or more sites before the droplet touches the second surface, independently of the system size. Thus, in Fig. 4 we plotted the numerical value of h in which the bridge is formed, shifted by 3 sites ($2h = 2h_c - 3$) and $h_{\min}$ against the system size. The plotted error bar represents the size of a lattice unit normalized by $\Omega^{1/3}$ and it decreases with system size. As the size of the system increases, the numerical value converges to the analytical expected value.

We can consider that the analytical and statistical liquid bridge models are composed of three kinds of elements: the planes, the liquid, and the vapor. However, these objects have a different treatment in each model: in the analytical model they are continuous and are described by the surface tension in the interface between the elements; in the statistical model they are composed of particles and are described by the interaction of each particle with its neighbors. During the process of liquid bridge rupture [22], we found almost no finite size effects because the liquid bridge is formed and the whole system is almost continuous, so a single site makes a negligible effect; see Fig. 3(c). However, during the process of the liquid bridge formation, we found a three-sites-effect which should only be neglected for very large systems. In other words, a single vapor particle between the droplet wall gap can make a difference; see Fig. 3(b).

In Fig. 5 we plot the free energy in both situations, when we reduce the distance between the planes to form the liquid bridge (filled square) and when we separate (open circles) the planes until the liquid bridge breaks. We compare these numerical simulations with the analytical solution (red line) [22]. We can observe a hysteresis curve with two gaps in the free energy. The vertical red lines correspond to the height at the formation of the liquid bridge, $h_{\min} = 0.25$, and at the rupture, $h_{\max} = 0.68$, computed analytically using Eqs. (2) and (9), respectively. The two gaps in the free energy indicate a possible mechanism for crackling sound generation in the lung during the inspiratory and expiratory breathing mechanics [1,23]. From both analytical and numerical models we calculate the total free energy released during both the formation and rupture of liquid bridges between two parallel planes. In both models, the formation has a greater loss of free energy than the rupture. In contrast, the experimental observations of Vyshedskiy, in real human airways, showed the opposite results. However, in real experimental data, the generated crackle sound waves are transmitted from the generation site through the parenchyma until they reach the skin, where they are captured by an electronic stethoscope. During this process, several frequencies are attenuated as the chest and transducers work as coupled acoustic filters [17,30–32]. We hypothesize that the inspiratory crackle has lower frequencies and some of them are absorbed during the transmission; this hypothesis is supported by the experimental data [1]. Another difference is the topology. The study of Vyshedskiy and the stress relaxation quadrupole theory considers a cylindrical geometry, while our model used two parallel planes.

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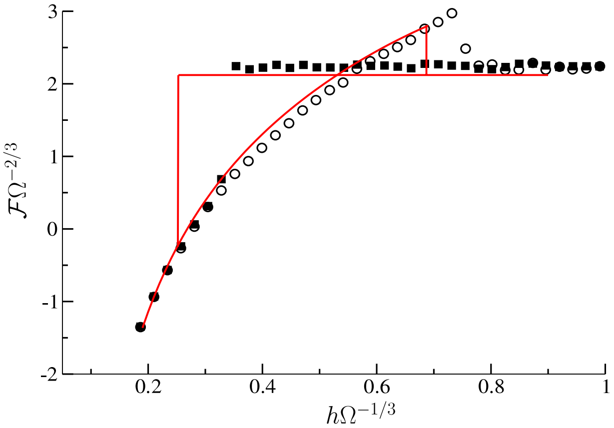

Fig. 5. The normalized total free energy $\mathcal{F}\Omega^{-2/3}$ versus the normalized half distance $h\Omega^{-1/3}$ during liquid bridge formation (filled squares) and liquid bridge rupture (open circles). The vertical red lines represent the values of $h_c = 0.687$ and $h_{\min} = 0.247$ obtained analytically [22]. The continuous red lines are the analytical calculation of the normalized total free energy $\mathcal{F}\Omega^{-2/3}$ for the liquid bridge and for the droplet. Here we use $\Theta \approx 50°$, 10 000 particles of liquid and lattice size of $60 \times 60 \times 52$. The hysteresis in energy highlights the two regions of instability, when we stretch the bridge or compress the droplet. Each point in the curve is an average of ten simulations.

Moreover, the continuous decrease in free energy as h decreases will generate an attractive force between the two planes [33]. Our simulation is quasistatic, meaning that we move the upper plane by one step down and wait until the system reaches equilibrium. Since the plane remains in a fixed position at each step until moving to the next step, there is an external force F_e, which is equal to the resultant force due the surface tension of the liquid bridge. Applying thermodynamics, we relate the force to the partial derivative of the potential energy with respect to the distance:

$$F_e = -\frac{1}{2}\left(\frac{\partial U}{\partial h}\right)_T + T\left(\frac{\partial F_e}{\partial T}\right)_h . \qquad (10)$$

We analyze the second term of Eq. (10), which is related to the entropy of the system. We numerically estimate it by calculating the force at two different temperatures and constant height. We verify that this term is very small and can therefore be neglected. Thus, for a fixed distance h, and volume Ω, we can write the external force, neglecting the entropic term, as

$$f = -\frac{\partial U}{2\partial h}. \qquad (11)$$

In Fig. 6, we show f computed from the liquid bridge energy and normalized half distance for three contact angles $\Theta = 39°$, $50°$, and $66°$. The result we obtained is analogous to the analytical calculations obtained in the literature for a contact angle $\theta > 30°$ [22,33]. We can notice that the force increases as h decreases, which leads to the collapse of the space between the planes as observed in flexible tubes. We can interpret the calculated force shown in Fig. 6 as the force needed to reopen a collapsed airway. This force is very high for small half distances h and decreases as we increase h. Therefore, once the external force pulling the planes apart becomes larger, the force attaching the planes to the bridge decreases and the bridge loses its stability.

3. Conclusions

From Fig. 1 we show the free energy difference between the two states, before and just after the liquid bridge formation, $\Delta\mathcal{F}$. The abrupt release of this energy causes mechanical instabilities and generates the bursting crackle sound. We can notice from Fig. 1 that $\Delta\mathcal{F}$ increases as Θ decreases, which may also correspond to the change in the pulmonary crackles strength as the properties of coating fluids change with the progression of the disease. The connection between the surface properties of the fluids in the lung and the crackle sound generated during the liquid bridge rupture or formation is crucial for understanding the pathology of several respiratory diseases and for improving clinical diagnosis [9,34]. However, our model in its present state cannot be directly applied to lung physiology mainly due the topological differences between our study and the real liquid bridge in the airways. In fact, in our model the liquid bridge forms between two planes, while in real airways the bridges block the cylindrical tubes.

We can also notice that the liquid bridge in the airways will form not only due to geometrical contraction of the airways, but also due to pressure fluctuations in airflow. It is known from the Bernoulli theory that the air flow reduces local hydrostatic pressure in proportion to the velocity squared. In a flexible tube, if a given region has a smaller diameter, the local pressure at that point has even lower pressure since the velocity increases inverse proportionally to the cross-section area. The lung airways are not only flexible, but also coated with a liquid layer which can easily move to the lower pressure

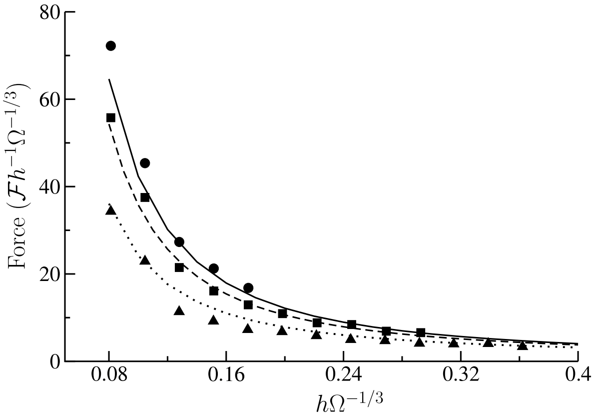

Fig. 6. The force between the planes for three different contact angles Θ computed using Eq. (11). Circle, square and triangle represent Θ equal to 39°, 50°, and 66°, respectively. The continuous, dashed and dotted lines are the analytical calculation force using Eq. (8) for Θ equal to 39°, 50°, and 66°, respectively. We use a lattice size of $60 \times 60 \times 52$ and 10 000 liquid particles.

regions generating instabilities and leading to airway closure. In addition, a complex mixture of organic fluids coating the airways may not be treated as a Newtonian fluid. Thus, a direct comparison between the energy released during the rupture of liquid bridges in the lung's airways and the system which we use here is not straightforward. However, our numerical algorithm can easily be implemented in arbitrary geometries, for example, the cylindrical geometry of bronchioles, since it is a standard lattice gas model with low computational cost. The main conclusion of this study is that our hypothesis that the expiratory crackles are generated by liquid bridge formation is a plausible one. Another conclusion is that the numerical model gives accurate results in a situation when it can be tested analytically and thus can be reliably used in more complex situations where analytical solutions are not possible.

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