Depletion interaction between two ellipsoids

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The depletion interactions between two ellipsoids in three configurations were studied by both Monte Carlo simulation with the Wang-Landau algorithm and the density functional theory in the curvature expansion approximation. Common features of the depletion interactions were found and the results were as expected. By comparing the results of the two methods, it is concluded that density functional theory under the curvature expansion approximation gave very good results to the depletion forces.
I. INTRODUCTION

Since the work of Asakura and Oosawa (AO) who pointed out that two hard spheres attract each other when suspended in a polymer solution based on the exclude volume argument over half a century ago, the researches on the depletion interactions in colloidal suspensions and in polymer-colloid systems are of longstanding and continuing interest. As we now understood, AO model is in fact the first order approximation in the density of the small component, which was polymer coils in AO’s theory. Mao et al extended the AO model to second- and third-order contributions of the small-particle density, where a repulsive potential barrier was found at separations next to the attractive potential. In subsequent studies, the depletion interactions of some relatively simple models, induced by a fluid of small hard spheres, have been studied in detail in theory, simulations, and experiments, including interactions between two spheres or a sphere near a wall. In recent years, complex models were also studied. The depletion interactions of big anisotropic objects including a hard rod or a hard ellipsoid near a planar wall or two hard spherocylinders have been calculated. Apart from the depletion interactions induced by fluids of small spheres, researches has also been performed to understand the depletion interaction induced by non-spherical colloidal suspensions. König studied the depletion force between non-spherical objects by extending the insertion approach of Roth. Depletion potentials in colloidal mixtures of spheres and rods have been studied by using the density functional theory (DFT) and Monte Carlo simulations. Very recently, Jin and Wu proposed a hybrid MC-DFT Method for studying depletion interactions, and used it to capture the entropic force between asymmetric particles.

The depletion interaction between nonspheric objects and induced by non-spheric suspensions are important for the real systems where depletion interaction play a role are mostly consisting of non-spheric objects. The shape of the ellipsoid may represent a large class of non-spheric objects range from a needle to a plate by changing the geometric parameters. Thus in this study we will focus on the depletion interaction of a simpler problem of two rotational ellipsoids in small sphere fluid system and try to get a deeper understanding of the nature of depletion.

In this paper, we consider the model of two hard rotational ellipsoids in a fluid of small hard spheres. The Monte Carlo simulation with Wang-Landau sampling is used to calculate...
the depletion potentials. Depletion toques are obtained by numerical differentiating the depletion potential with respect to angles. We also employed the DFT approach to calculate the depletion potential to compare with our simulation results.

The relevant details of the models we consider in this work are given in Sec. II. The implementation of Wang-Landau sampling in our simulation is presented in Sec. III. In Sec. IV DFT approach under curvature expansion is described. In Sec. V, we present the simulation results, and compare with the results obtained by DFT approach. Finally, we conclude the whole paper in Sec. VI.

II. DEFINITION OF THE TYPICAL CONFIGURATION

The system we shall investigate consists of two rotational ellipsoids immersed in a hard sphere fluid, one of the ellipsoids is in a fixed position, by changing the separation and orientation of the second ellipsoid with the first one and calculating the depletion forces in each configuration, the full depletion force between the two ellipsoid can be obtained. There are four degrees of freedom in this system, the full calculation amount to scan discretized points in four dimensions, which is a task too heavy to be done at the present computation power. Thus we choose three typical configurations to study, each of which is specified by a pair of degrees of freedom, and the three configurations can give a scratch or overall view of the full depletion force. The unit of length in calculation is the diameter of the small spheres. The ellipsoid is specified by its long axis $2A$ and short rotational axis $2B$, and in the following the long axis of the fixed ellipsoid is along the $x$ axis. The first configuration (referred to as C-1 hereafter) is to put the long axis of the second ellipsoid parallel to the first one, with its center shifted $x_{\parallel}$ in $x$ direction to the center of the first one, and separated $h+2B$ in $z$ direction. Thus the two ellipsoids located at the positions $\left(-\frac{x_{\parallel}}{2},0,-\frac{(2B+h)}{2}\right)$ and $\left(+\frac{x_{\parallel}}{2},0,\frac{(2B+h)}{2}\right)$ respectively. The depletion potential $W(x_{\parallel},h)$ between these two hard ellipsoids is a function of the shift $x_{\parallel}$ and the separation $h$ in $z$ direction. The size of the simulation box is $L_x \times L_y \times L_z$ with $L_x = 2A + x_{\parallel} + 8\sigma, L_y = 2B + 8\sigma$ and $L_z = 4B + h_{\text{max}} + 8\sigma$ respectively. $h_{\text{max}}$ is the maximum value of $h$ in our calculation. The choice of simulation box is according to Dickman, which is large enough to neglect finite size effects safely when volume fraction of the small spheres is less than 0.3. The volume fraction of small spheres is defined by $\eta_s = N\pi\sigma^3/6/V_{\text{eff}}$ and $V_{\text{eff}} = L_x \times L_y \times L_z - 2V_{\text{ellipsoid}}, V_{\text{ellipsoid}} = \frac{4}{3}\pi AB^2$.
respectively. Periodic Boundary conditions are applied to all three space directions.

The second configuration (referred to as C-2 hereafter) is that the second ellipsoid placed \( h + 2B \) away along the \( z \)-axis from the first one, and the long axes is rotated about \( z \) axis by an angle \( \theta \). The two unit vectors along each long axis are \((\sin\left(-\frac{\theta}{2}\right), \cos\left(-\frac{\theta}{2}\right), 0)\) and \((\sin\left(+\frac{\theta}{2}\right), \cos\left(+\frac{\theta}{2}\right), 0)\) respectively. The centers of mass of the two hard ellipsoids are located at \( \left(0, 0, -\frac{(2B+h)}{2}\right) \) and \( \left(0, 0, \frac{(2B+h)}{2}\right) \) respectively. The size of the simulation box is \( L_x \times L_y \times L_z \) with \( L_x = 2B + 2A \sin\left(\frac{\theta}{2}\right) + 8\sigma \), \( L_y = 2B + 2A \cos\left(\frac{\theta}{2}\right) + 8\sigma \) and \( L_z = 4B + h_{\text{max}} + 8\sigma \) respectively, chosen with the same criterion as that in C-1. The depletion potential \( W(\theta, h) \) depends on the angle \( \theta \) and the separation \( h \) of the two hard ellipsoids. The periodic boundary conditions are also applied to all three space directions.

The third configuration (referred to as C-3 hereafter) is specified by two parameters, the angle \( \Phi \) of the second ellipsoid rotated about \( y \) axis and minimal surface-to-surface distance \( h \) between two hard ellipsoids. For example, \( h = 0 \) when the two hard ellipsoids just contact each other. \( z_{\text{min}} \) and \( x_{\text{min}} \) depend on angle \( \Phi \) by \( z_{\text{min}} = \left(A^2 \sin^2\left(\frac{\Phi}{2}\right) + B^2 \cos^2\left(\frac{\Phi}{2}\right)\right)^{\frac{1}{2}} \) and \( x_{\text{min}} = \left(A^2 \cos^2\left(\frac{\Phi}{2}\right) + B^2 \sin^2\left(\frac{\Phi}{2}\right)\right)^{\frac{1}{2}} \) from simple geometric considerations. When \( h \) and \( \Phi \) are given, the locations of the two hard ellipsoids are at \( \left(0, 0, -(2z_{\text{min}}+h)\right) \) and \( \left(0, 0, \frac{(2z_{\text{min}}+h)}{2}\right) \). The unit vectors along each hard ellipsoid are \((\cos\left(\frac{\Phi}{2}\right), 0, \sin\left(\frac{\Phi}{2}\right))\) and \((\cos\left(-\frac{\Phi}{2}\right), 0, \sin\left(-\frac{\Phi}{2}\right))\). According to the same criterion as the first two configurations, the simulation box size is chosen to be \( L_x \times L_y \times L_z \) with \( L_x = 2x_{\text{min}} + 8\sigma \), \( L_y = 2B + 8\sigma \), \( L_z = 4 \times z_{\text{min}} + h_{\text{max}} + 8\sigma \). The periodic boundary conditions are used in three space directions.

### III. METHOD OF CALCULATION

#### A. Monte Carlo Simulation

We describe the simulation method here. The depletion potential for a given configuration of the two ellipsoids is the free energy of the whole system under such a configuration, we may chose the zero point of the depletion potential when the two ellipsoids are infinitely separated. Thus what we need to calculate is the free energy difference of a configuration with that of infinite separation. There are different schemes in literatures in the evaluation of the free energy difference by Monte Carlo simulations. Here we adopt the Wang-Landau method. The method was first proposed by Wang and Landau\(^{18} \) with lattice models to calculate
the energy density of states, and extended to off-lattice systems by Shell. The efficiency
and robustness of the Wang-Landau sampling algorithm in estimation of the density of
state (DOS) are excellent in a wide range of model systems.

The system in this study consists of hard objects only, thus the internal energy is only
the kinetic energy which is determined by temperature only and irrelevant to the depletion
potential. The part that contributes to depletion potential is the variance of entropy of the
system with configurations and the entropy is directly related to the number of microscopic
states as $S = k_B \ln g$ where $g$ is the number of microscopic states of a given macroscopic
configuration. The depletion potential $W$ is given by

$$
\frac{W}{k_B T} = - \left( \frac{S}{k_B} - \frac{S_0}{k_B} \right) = - \ln \left( \frac{g}{g_0} \right).
$$

Here $S_0$ and $g_0$ are the entropy and number of microscopic states of the system when two el-
lopsoids infinitely separated, respectively. The ratio of the number of microscopic states can
be calculated directly from the Wang-Landau method. In the three macroscopic configura-
tions considered, each configuration was characterized by two parameters. The calculation
is proceeded in the following way: one parameter is fixed at several different values and the
second parameter is divided into small intervals, the microscopic density of states of the sec-
ond parameter is then evaluated by the Wang-Landau method and the depletion potential
is then calculated. For each fixed value of the first parameter, an independent run is needed.

The sampling of the simulation consists of two parts. The first part is the move between
ellipsoids configurations, the second ellipsoid moved in the one parameter intervals accord-
ing to the acceptance criterion $P(Stat{e}_\text{old} \rightarrow Stat{e}_\text{new}) = \min(1, g(Stat{e}_\text{old})/g(Stat{e}_\text{new}))$.
where $g(Stat{e})$ is the density of states of the current state, specified by the fixed first pa-
rameter and the current interval of the second parameter. When a state is visited, the
corresponding density of states $g(\text{state})$ is updated by multiply a factor $f$. The second part
is the sampling of the small hard spheres when an ellipsoids configuration is specified, the
Metropolis sampling is used in this part, i.e. a randomly chosen small hard sphere with a
random trial move is accepted if the move does not result an overlap with other objects. For
each move of the ellipsoid, usually $10^5$ Monte Carlo steps of the small hard sphere system
were performed in order to keep the equilibrium. The initial value of $f = f_0$ is chosen to be
$e^{0.01}$ in our simulation, which is different with the common value $e^1$, simply because the free
energy landscape of depletion is relatively flat compared with other systems. Accumulated
histogram $H(state)$ are updated during the random walk. When $H$ is flat, we clear $H$ and modify $f$ to $f^{1/2}$. The whole simulation stopped when the modification factor smaller than $\exp(10^{-8})$.

B. DENSITY FUNCTIONAL THEORY

In this section we describe the density functional theory (DFT) method used in this study. The DFT is a very efficient theoretical method for the calculation of depletion interactions. The basics of the method is to take the two ellipsoid as external potential of the small hard sphere systems and finding the density distribution and free energy of the small hard sphere system by the minimization of the free energy functional. For hard sphere systems the fundamental measure theory (FMT) proposed long time ago by Rosenfeld and its various extensions and modifications usually gave pretty accurate values of free energy. However, the minimization of the free energy functional in the general three dimension is computationally heavy and, in some cases even impractical. In real calculations one often reduce the problem to two dimensional or even one dimensional by symmetry of the system studied. In the depletion potential calculation, the so called insertion approach proposed by R. Roth et al is a very effective way to reduce the dimensionality. In this approach only one solute particle is fixed so that higher symmetry usually available and thus it can drastically reduce the computation load.

In the insertion approach the depletion potential is related to the one body direct correlation function $C_b^{(1)}(r, \omega)$ as

$$\beta W(r, \omega) = C_b^{(1)}(|r| \to \infty, \omega) - C_b^{(1)}(r, \omega),$$

the direct correlation function can be calculated within FMT framework by

$$C_b^{(1)} = -\sum_{\alpha} \frac{\partial \Phi}{\partial n_{\alpha}} \otimes \omega_{\alpha}^b.$$  

Here $\Phi$ is a function of the weighted density $\{n_{\alpha}(r)\}$, given by

$$\Phi(\{n_{\alpha}(r)\}) = -n_0 \ln(1 - n_3) + \frac{n_1 n_2 - n_1 \cdot n_2}{1 - n_3} + \frac{n_3^2 - 3n_2 n_2 \cdot n_2}{24\pi (1 - n_3)^2}$$

where $\{n_{\alpha}\}$ are weighted densities of four scalar types and two vector types given by:

$$n_{\alpha}(r) = \int \omega_{\alpha}^{(r - r')} \rho(r') \, dr', \quad \alpha = 0, 1, 2, 3$$
\( n_\alpha (r) = \int \omega_\alpha \left( r - r' \right) \rho \left( r' \right) \, d r', \quad \alpha = 1, 2. \) \hspace{1cm} (5)

The weight functions for spherical hard body are given by

\( w_3 (r) = \Theta \left( |r - R_b (\theta, \phi)| \right) \) \hspace{1cm} (6)

\( w_2 (r) = \delta \left( |r - R_b (\theta, \phi)| \right) \) \hspace{1cm} (7)

\( \omega_1 (r) = \frac{\omega_2}{4\pi R} \) \hspace{1cm} (8)

\( \omega_0 (r) = \frac{\omega_2}{4\pi R^2} \) \hspace{1cm} (9)

\( w_2 (r) = -\nabla \omega_3 (r) = n_b (r) \delta \left( |r - R_b (\theta, \phi)| \right) \) \hspace{1cm} (10)

\( w_1 (r) = \frac{w_2 (r)}{4\pi R^2} \) \hspace{1cm} (11)

In our system, under the insert particle scheme, the fixed solute is a rotational ellipsoid, a full calculation requires the minimization of the free energy functional on a two dimensional grid, which is still computationally heavy if the grid is refined to reach the required accuracy. If it can be further reduced to a one dimensional problem, then the calculation will be much easier to accomplish. In a recent work\(^ {21}\), König et al. presented an ansatz for the density profile of small particles around a big fixed object:

\[ \rho_s (r) = \rho_s^P (u) + H (R) \rho_s^H (u) + K (R) \rho_s^K (u) + \cdots \] \hspace{1cm} (12)

\( r \) is the point outside the fixed object, \( R \) is the closest point from \( r \) on the surface of the fixed object where \( \rho_s (r) \) vanishes. \( R - r = u n (R) \), \( n (R) \) is the unit vector normal to the surface at point \( R \). \( H \) and \( K \) are the mean and Gaussian curvature at point \( R \). Based on this assumption, König et al. then introduced the curvature expansion approximation for studying depletion force between two nonspherical objects\(^ {14}\). They further argue that \( \Psi_\alpha (r) \) for one fixed object can be expanded by the surface curvature of the object

\[ \Psi_\alpha (r) = \Psi_\alpha^P (u) + H (R) \Psi_\alpha^H (u) + K (R) \Psi_\alpha^K (u) + \cdots \] \hspace{1cm} (13)

where \( \frac{\partial \Phi}{\partial m_\alpha} = \Psi_\alpha \). Under this approximation, we only need to calculate \( \Psi_\alpha (r) \) near simple geometry objects to get \( \Psi_\alpha^P (u) \), \( \Psi_\alpha^H (u) \), and \( \Psi_\alpha^K (u) \). And then \( \Psi_\alpha (r) \) near nonspherical object can be obtained.
In order to obtain the convolution of $c^{(1)}_b$ for the insertion of second nonspherical object, Rosenfeld’s generalized FMT for convex hard bodies\(^{22}\) is employed as Roth’s previous application in the calculation of the depletion torque\(^ {11}\). The weight functions are

\[ w^b_3 (r) = \Theta(|r - R_b (\theta, \phi)|) \quad (14) \]

\[ w^b_2 (r) = \delta(|r - R_b (\theta, \phi)|) \quad (15) \]

\[ \omega^b_1 (r) = \frac{H (r)}{4\pi} \omega^b_2 \quad (16) \]

\[ \omega^b_0 (r) = \frac{K (r)}{4\pi} \omega^b_2 \quad (17) \]

where $H(r)$ is the mean curvature of the second object, and $K(r)$ is the Gaussian curvature of the second object.

\[ w^b_2 (r) = -\nabla \omega^b_3 (r) = n_b (r) \delta(|r - R_b (\theta, \phi)|) \quad (19) \]

where $n_b (r)$ is the unit vector normal to the surface at point $r$, and

\[ w^b_1 (r) = \frac{H (r) w^b_2 (r)}{4\pi} \quad (20) \]

**IV. RESULTS AND COMPARISON**

We carried out calculations both with Monte Carlo simulations and DFT method described in the previous section for the three configurations defined in section \[\text{III}\].

Figure 1(a) shows the Monte Carlo simulation results of the variation of depletion potential $\beta W (x, h)$ with $h$ for different fixed $x$ of the configuration $C=1$. The parameters for the ellipsoids are $A = 5\sigma$ and $B = 0.5\sigma$. The volume fraction of small hard spheres is $\eta_s = 0.3$. The curves are the variations of the depletion potential with the separation between the ellipsoids, each curve corresponding to a fixed value of $x$. For clarity reasons, all the potential curves are shifted so that their potential zero at the point $(x, 0)$. From the figure we see that the depletion force is much stronger when the centers of the two ellipsoids are not shifted with each other, and becomes weaker when the shift becomes larger.
FIG. 1. (a), The depletion potential of configuration C-1, $A = 5\sigma$, $B = 0.5\sigma$, the volume fraction of small hard spheres is $\eta_s = 0.3$. Each curve corresponding to one $x_\parallel$ and all curves are shifted so that the $W(x_\parallel,0) = 0$ for clarity. (b), The variation of depletion potential $W(x_\parallel,0)$ with respect to $x_\parallel$.

The properties of the depletion force is similar with different shifts and also similar to the depletion potential between two hard spheres, i.e, the depletion force is attractive at small separations and then turn to repulsive at a separation about the diameter of small hard spheres, and oscillates slightly afterwards then tends to zero. This is a typical feature of depletion. Figure 1 (b) is the variation of the depletion potential with the shift $x_\parallel$ at $h = 0$, it is precisely the relative shift value of each curve in figure 1 (a). The curve is relative flat in the regions $x_\parallel < 1$ and $x_\parallel > 8$. In the first case the two ellipsoid are only shifted slightly and the influence of the shift is small, and in the second case the shift is so large that the two ellipsoids are already well separated in the $x$ direction thus further shift only has very small effect on the depletion potential. In the middle part the shift changes the depletion domain (the region of space that the small hard spheres are unable to enter) between the two ellipsoids thus changes the depletion potential.

Figure 2 (a) are the variation with the separation $h$ of the depletion potential $\beta W(\theta,h)$ for different fixed rotation values of $\theta$. The other parameters are the same as the figure 1. For clarity reasons the curves are shifted so that the potential at $h = 0$ coincide and set to zero for different $\theta$’s. It is clear that the depletion force in the cases of small $\theta$ is much stronger than those of large $\theta$, which is the reflection of the fact that for the long ellipsoids studied here, small $\theta$ means strong depletion and results larger depletion force. The variation
FIG. 2. (a) The depletion potential $W(\theta, h)$ of configuration C-2. Each curve corresponding to a fixed value of rotation angle $\theta$, the curves are shifted so that the zero of the potential is at point $h = 0$, other parameters are the same as the figure 1. (b) The variation of the depletion potential at $h = 0$ with the rotation angle $\theta$. (c) The depletion torque between the two ellipsoids obtained from numerical differentiation of the depletion potential for $h = 0$.

The depletion potential $W(\theta, h = 0)$ with rotation angle $\theta$ at $h = 0$ is given in figure 2 (b). It varies strongly in the small $\theta$ region and tends to be flat for large $\theta$ as expected. Figure 2 (c) is the depletion torque at $h = 0$ obtained from numerical differentiation of the depletion potential as shown in figure 2 (b). The torque is less than zero which means it is a restoring torque as already clear from the depletion potential curve of figure 2 (b). This restoring torque is at its maximum at $\theta \approx 8^\circ$.

The depletion potential of the configuration C-3, $\beta W(\Phi, h)$ is shown in figure 3. Figure 3 (a) shows the variation of depletion potential with $h$ for several fixed $\Phi$’s. The other
FIG. 3. (a) The variation of depletion potential with $h$ for configuration 3 with different fixed values of $\Phi$, the curves are shifted in the same way as figure 1 and the parameters are also the same as figure 1 (b). The variation of depletion potential with $\Phi$ at $h = 0$. (c) The depletion torque at $h = 0$ as function of $\Phi$.

parameters are the same as in figure 1. The curves are shifted in the same way as figure 1 and 2 so that the potential zero is at $h = 0$. The variation of the depletion potential with $\Phi$ at $h = 0$ is shown in figure 2 (b) and the depletion torque with respect to the $y$ axis, obtained from numerical differentiation of the figure 3 (b), is shown in figure 3 (c). As in the case of configuration C-2, the torque is negative and has the effect to restoring the configuration to the $\Phi = 0$ state.

Put together the results of all three configurations we can conclude that the minimum of the depletion potential is the state that two ellipsoids parallel in their long axis without shifting. When the two ellipsoids deviates from such a state the depletion force and depletion torque will restore the state. Since the three body depletion force and high order many body
depletion forces are very small compared to two body ones, it is expected that the depletion may play a crucial role for the self-assembly of ellipsoids system to form nematic order when immersed in a small hard sphere system or in a solution with polymer blends.

Figure 4(a) — figure 4(c) are the comparisons of the DFT results under the curvature expansion approximation with the Monto Carlo results. Figure 4 is for the configuration C-1, where symbols are results from MC simulations and lines are from DFT method in the curvature expansion as described in section III B.

Figure 4(a) and Figure 4(b) show the comparisons of MC and DFT for configuration C-2 and configuration C-3 respectively. The agreement between DFT results and the corresponding simulation results are considerably good. As indicated by König, the most inaccurate part of the curvature expansion approximation is those region near the surface of the fixed object. Thus our model of two nearly parallel needle-like ellipsoids near each other
is a very harsh test situation for the approximation, since the near surface contribution is the main contribution of the whole integral. Even though, inaccuracy of the depletion well depth obtained by the DET under curvature expansion approximation is less than 10%. Since the curvature expansion DFT method use much smaller computational resources compared to both the original FMT DFT method and the Monte Carlo simulation, and it is also easy to implement, it is an excellent method in the estimation of depletion forces for many different situations of non spherical objects.

V. SUMMARY

In summary, we calculated the depletion interaction of two hard ellipsoids in a fluid of small hard spheres by using Wang-Landau sampling Monte Carlo simulations and the density functional theory under curvature expansion. Our simulation suggests that Wang-Landau sampling is an efficient method for calculating the depletion potential of two ellipsoids, and the curvature expansion DFT approach is a much computationally cheaper yet considerably accurate theoretical method compared with the simulation ones. Instead of an investigation of the depletion potential in the whole parameter space, which is both unnecessary and impractical for its heavy computation load, we have revealed the key aspects of depletion interactions in this system by choosing the three representative configurations.

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