New Physics: Sae Mulli,
Vol. 69, No. 9, September 2019, pp. 932∼938
http://dx.doi.org/10.3938/NPSM.69.932

Statistical Mechanics and Information Theory

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(Received 21 March 2019 : revised 14 June 2019 : accepted 22 July 2019)

We present a different formulation of statistical mechanics from the perspective of information theory and apply the formalism to a simple system as a concrete example. This is accomplished by decomposing the Shannon entropy and mutual information into their distinct components. We consider a small one-dimensional thermodynamic system interacting with a hard-sphere potential. We can explicitly calculate the mutual information between two particles and triple mutual information among three particles as functions of the volume fraction of the system. We also examine the effect of boundary conditions on the mutual information.

PACS numbers: 02.50.CW, 05.20.−y, 89.70.−a, 89.70.cf
Keywords: Probability theory, Classical statistical mechanics, Information theory, Mutual information

I. Introduction

Information is now becoming widespread as an essential element in describing the physical world around us after Landauer declared a famous sentence "Information is physical" in 1991 [1]. Wheeler [2] also suggested that our experiences of objects or phenomena that constitute reality are the results of binary decisions which we do in the process of observing them. Thus he aesthetically coined a phrase "It from bit". But there are still more controversies in this issue than settled [3–5]

A noninteracting system or ideal gas system is completely independent between the constituent particles, and thus the mutual information between them is identically zero for any thermodynamic states. However, for an interacting system, interaction induces mutual information between them. Our question here is: How much mutual information do we get for a given thermodynamic system? It may depend on not only the potential model employed but also the thermodynamic state of the system. For this purpose, we will formulate a new statistical mechanics in terms of the information theory [6–8]

Shannon entropy [9] of a continuous system with a probability density $P(x)$ is defined by

$$H(X) \equiv -\int P(x) \ln P(x) dx, \tag{1}$$

which measures the inherent uncertainty of a continuous random variable X. This differential entropy may have a negative value and/or diverge due to arbitrary smallness of the probability density function $P(x)$. But, the difference in Shannon entropy cancels the divergence so that it becomes finite. This is the reason why we decompose the Shannon entropy.

Here, we will explicitly calculate it for a hard-sphere potential model, as an example. Fortunately, we obtain exact results for small systems. In Sec. II, we first present a review of information theory. Next, in Sec. III, we formulate classical statistical mechanics of a thermodynamic system in terms of information theory and then decompose into distinct components of the entropy and the mutual information. In Sec. IV, in order to see the effectiveness of the formalism, we apply it to a small thermodynamic system under a hard-sphere interaction. Because the system is small, we should also include the effect of boundary conditions of the system. We explicitly calculate mutual information between two particles and triple mutual information among three particles as a function of volume fraction η. We find that the triple mutual information among three particles under hard-sphere interaction shows only a synergy effect under fixed wall boundary condition, but under periodic

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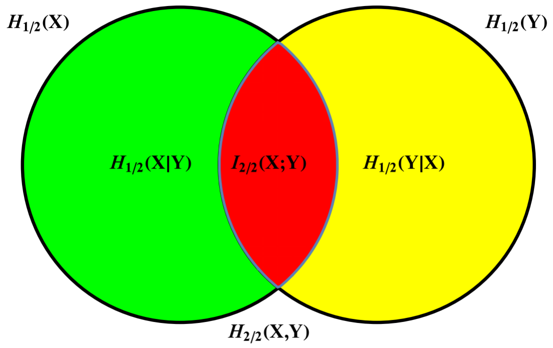
boundary condition, it changes from synergy to redundancy in higher densities. Finally, in Sec. V, we conclude this article.

II. Information Theory

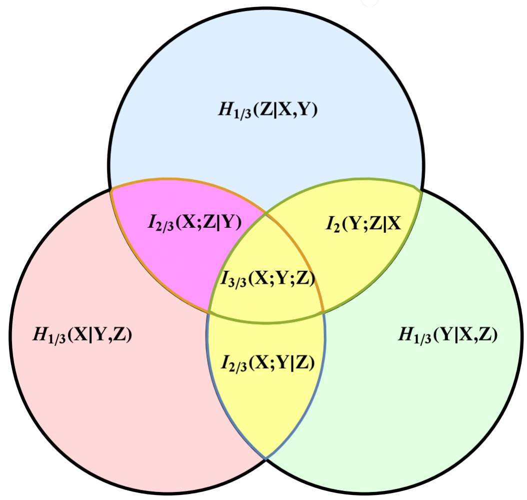
In order to introduce necessary notations, we first review information theory. Upper case letter (e.g. X, Y) denotes a random variable and its lower case (e.g. x, y) corresponds to a possible value of this random variable. The Shannon entropy $H(X)$ defined in Eq. (1) is to measure the uncertainty in a realization of X. Let $P_{2/2}(X,Y)$ be the joint probability distribution of occurrences of random variables X and Y. Shannon entropy for the joint probability is defined by $H_{2/2}(X,Y) = -\int P_{2/2}(x,y) \ln P_{2/2}(x,y) dxdy$. The joint entropy $H_{2/2}(X,Y)$ measures how much uncertainty there is in the two random variables X and Y considered together. The marginal distributions are defined by $P_{1/2}(x) = \int P_{2/2}(x,y)dy$ and $P_{1/2}(y) = \int P_{2/2}(x,y)dx$, respectively.

Now, we want to quantify how much uncertainty does a random variable X have if another random variable Y is known. We define the conditional entropy as $H_{1/2}(X|Y) = -\int P_{2/2}(x,y) \ln \frac{P_{2/2}(x,y)}{P_{1/2}(y)} dxdy$, measuring, on average, how much uncertainty remains in X if we know Y. The conditional probability is defined by $P_{1/2}(y/x) = \frac{P_{2/2}(x,y)}{P_{1/2}(x)}$. It is easy to see that the conditional entropy can be written as $H_{1/2}(X|Y) = H_{2/2}(X,Y) - H_{1/2}(Y)$, a kind of chain rule. If X = Y, then $H_{1/2}(X|Y) = 0$. The inequality $H_{1/2}(Y) \leq H_{1/2}(X,Y)$ seems to be intuitive, as the uncertainty of the whole has to be at least as big as the uncertainty of a part.

Information diagram is a Venn diagram for various information measures. As shown in Fig. 1a, the area contained by both circles is the joint information $H_{2/2}(X,Y)$. The circle on the left (red and green) is the individual information, $H_{1/2}(X)$, with the green being the conditional entropy $H_{1/2}(X|Y)$. The circle on the right (yellow and red) is $H_{1/2}(Y)$, with the yellow being $H_{1/2}(Y|X)$. The red is the mutual information $I_{2/2}(X;Y)$, that measures the common uncertainty between X and Y, defined by



(a) Joint entropy, conditional entropy and mutual information of two events X and Y. There are 3 disjoint components.



(b) Triple mutual information of three events X,Y and Z. There are 7 disjoint components.

Fig. 1. (Color online) Information diagram.

$$I_{2/2}(X;Y) \equiv \int P_{2/2}(x,y) \ln \frac{P_{2/2}(x,y)}{P_{1/2}(x)P_{1/2}(y)} dxdy$$
$$= H_{1/2}(X) + H_{1/2}(Y) - H_{1/2}(X,Y)$$
$$= H_{1/2}(X) - H_{1/2}(X/Y).$$

Now, let us examine the triple mutual information for three random variables X, Y and Z, as shown in Fig. 1b. The conditional mutual information $I_{2/3}(X;Y|Z)$ is the expected value of the mutual information of two random variables X and Y, given the value of a third Z, defined by

$$I_{2/3}(X;Y|Z) \equiv \int dz P_{1/3}(z) \int dxdy P_{2/3}(x,y|z) \times \ln \frac{P_{2/3}(x,y|z)}{P_{1/3}(x|z)P_{1/3}(y|z)}.$$

It is a measure of how much uncertainty is shared between X and Y, but not in Z. Alternatively, we can also write in terms of joint entropy and conditional entropy as

$$\begin{aligned} I_{2/3}(X;Y|Z) &= H_{2/3}(X,Z) + H_{2/3}(Y,Z) \\ &\quad - H_{3/3}(X,Y,Z) - H_{1/3}(Z) \\ &= H_{1/3}(X|Z) - H_{1/3}(X|Y,Z). \end{aligned}$$

Triple mutual information among three random variables (X, Y, Z) is defined as $I_{3/3}(X;Y;Z) \equiv I_{2/3}(X;Y) - I_{2/3}(X;Y|Z)$ where $I_{2/3}(X;Y)$ is mutual information between X and Y in three variables (X,Y,Z). In words, $I_{3/3}(X;Y;Z)$ is the difference between information shared by (X,Y) given information on Z and without information on Z. Or, it is the influence of Z on the amount of information shared between (X, Y). It can also be written

$$\begin{aligned} I_{3/3}(X;Y;Z) &= I_{2/3}(X;Z) - I_{2/3}(X;Z|Y) \\ &= I_{2/3}(Y;Z) - I_{2/3}(Y;Z|X). \end{aligned}$$

It has a value [10] in the range of

$$\begin{aligned} &- min(I_{2/3}(X;Y|Z), I_{2/3}(Y;Z|X), I_{2/3}(X;Z|Y)) \\ &\leq I_{3/3}(X;Y;Z) \\ &\leq min(I_{2/3}(X;Y), I_{2/3}(Y;Z), I_{2/3}(X;Z)). \end{aligned}$$

Thus, $I_{3/3}(X;Y;Z)$ can have positive, zero or negative values. Let us consider three cases separately. Rather trivial case is $I_{3/3}(X;Y;Z) = 0$, if all the random variables are completely independent of each other. In other words, if the dependency between (X, Y) is due entirely to the influence of Z, then $I_{3/3}(X;Y;Z) = 0$. If Z inhibits the correlation between (X, Y), then $I_{3/3}(X;Y;Z) > 0$. This case is called redundancy. If Z enhances the correlation between (X, Y), then $I_{3/3}(X;Y;Z) < 0$. This case is called synergy. Synergy means that if working together two or more parts of a system, the combined effect is greater than the sum of the effects of the parts. Actually, $I_{3/3}(X;Y;Z)$ measures the intrinsic three-body contribution, not originated from the two-body contribution.

III. General Formulation of Statistical Mechanics in Terms of Information Theory

Let us consider a thermodynamic system composed of N identical particles confined in a cubic volume $V = L^3$. The system is contacting with a heat reservoir at temperature T and so it can be described in terms of canonical ensemble. The potential energy of the system is assumed to be a sum of pair potentials $\phi(r)$, $u_N\left(\vec{q}_1, \cdots, \vec{q}_N\right) = \sum_{i>j}^N \phi\left(\left|\vec{q}_i - \vec{q}_j\right|\right)$. The configurational energy of the system is given by $U_N = \left\langle u_N\left(\vec{q}_1, \cdots, \vec{q}_N\right)\right\rangle$ where $\langle\cdots\rangle$ denotes an ensemble average. The configurational partition function is defined by

$$Q_N \equiv \int_0^V \cdots \int_0^V e^{-\beta u_N\left(\vec{q}_1, \cdots, \vec{q}_N\right)} d\vec{q}_1 \cdots d\vec{q}_N,$$

where $\beta = 1/kT$ is the inverse temperature with k the Boltzmann's constant. If we scale each coordinate $\vec{q}_i$ with L as $\vec{x}_i \equiv \frac{\vec{q}_i}{L}$, then we have $Q_N = \nu_N V^N$, where

$$\nu_N \equiv \int_0^L \cdots \int_0^L e^{-\beta u_N\left(L\vec{x}_1, \cdots, L\vec{x}_N\right)} d\vec{x}_1 \cdots d\vec{x}_N$$

which is a ratio of available configurational hypervolume of the system.

The configurational probability density to find N particles located at $\left(\vec{q}_1, \cdots, \vec{q}_N\right)$ is given by

$$P_{N/N}\left(\vec{q}_1, \cdots, \vec{q}_N\right) = \frac{e^{-\beta u_N\left(\vec{q}_1, \cdots, \vec{q}_N\right)}}{Q_N} \tag{2}$$

and the corresponding Shannon information is written as

$$H_{N/N} = -\int_0^V \cdots \int_0^V P_{N/N} \ln P_{N/N} d\vec{q}_1 \cdots d\vec{q}_N.$$

The n-th reduced probability density function for the N-particle system is defined by [11]

$$P_{n/N}\left(\vec{q}_1, \cdots, \vec{q}_n\right) \equiv \frac{\int_0^V e^{-\beta u_N\left(\vec{q}_1, \cdots, \vec{q}_N\right)} d\vec{q}_{n+1} \cdots d\vec{q}_N}{Q_N}, \quad n = 1, 2, \cdots, N-1. \tag{3}$$

Now, let us introduce auxiliary variables A and B for notational convenience. N-th reduced probability density function in Eq. 2 can be formally written as

$P_{N/N} = \frac{A_{N/N}}{L^N \nu_N}$, with $A_{N/N} \equiv e^{-\beta u_N\left(L\vec{x}_1,\cdots,L\vec{x}_N\right)}$ and the corresponding Shannon entropy is written as

$$H_{N/N} = \frac{B_{N/N}}{\nu_N} + N\ln L + \ln\nu_N.$$

Similarly, the n-th reduced probability density function in Eq. 3 is rewritten as $P_{n/N} = \frac{A_{n/N}}{L^n \nu_N}$, where

$$\begin{aligned} A_{n/N} &\equiv \int_0^1 \cdots \int_0^1 e^{-\beta u_N\left(L\vec{x}_1,\cdots,L\vec{x}_N\right)} d\vec{x}_{n+1}\cdots d\vec{x}_N \\ &= \int_0^1 A_{(n+1)/N} d\vec{x}_{n+1}. \end{aligned}$$

We then have a recurrence relation for $A_{n/N}$, in reverse order, starting from N. Note that $A_{0/N} = \nu_N$. The reduced Shannon entropy is written as,

$$H_{n/N} = \frac{B_{n/N}}{\nu_N} + n\ln L + \ln\nu_N, \tag{4}$$

where

$$B_{n/N} \equiv -\int_0^1 \cdots \int_0^1 A_{n/N}\ln A_{n/N} d\vec{x}_1\cdots d\vec{x}_n.$$

Note that $B_{0/N} = -\nu_N\ln\nu_N$ and $B_{N/N} = \nu_N\beta U_N$, so that $H_{0/N} = 0$ and $H_{N/N} = N\ln L + \ln\nu_N + \beta U_N$.

The configurational part of thermodynamic entropy is given by $S_{conf} = \lim_{N\to\infty} kH_{N/N}$, connecting the Shannon entropy with thermodynamics.

Now, let us decompose the reduced Shannon information $H_{n/N}$ in Eq. (4). This can be done rather easily for $N = 2$ or 3. For N=2 case, as shown in Fig. 1a, we obtain

$$H_{1/2}(1|2) = -\frac{B_{1/2}}{\nu_2} + \ln L + \beta U_2,$$

$$I_{2/2}(1;2) = \ln\nu_2 - \beta U_2 + 2\frac{B_{1/2}}{\nu_2}.$$

Here, the number 1, for example, in parentheses denotes an abbreviation for the position $\vec{q}_1$ of the particle 1. Again, for N=3 case, as shown in Fig. 1b, the decomposed disjoint components can be written as

$$H_{1/3}(1|2,3) = -\frac{B_{2/3}}{\nu_3} + \ln L + \beta U_3,$$

$$I_{2/3}(1;2|3) = \frac{-B_{1/3} + 2B_{2/3} - B_{2/3}}{\nu_3},$$

$$I_{3/3}(1;2;3) = \ln\nu_3 + \beta U_3 + 3\frac{B_{1/3} - B_{2/3}}{\nu_3}.$$

IV. Application to a Hard Sphere System

For any pair potential $\phi(r)$, it is difficult to exactly calculate $A_{n/N}$ and $B_{n/N}$ for large N particle system. So we have to consider the small system size N in order to make it amenable. Thus, in order to obtain explicit analytic expressions, we restrict the number of constituent particles of the system to N=2 or 3. Hard sphere potential is one of the simplest potential we can think of. Hard sphere potential is defined by

$$u(r) = \begin{cases} \infty, & r \le \sigma, \\ 0, & \text{otherwise}, \end{cases}$$

where σ is the diameter of the hard sphere core. We also further restrict the system to one-dimension. In one-dimensional space, a single hard sphere particle can reduce a volume by an amount σ, so that the volume of the system is reduced by $N\sigma$ for N particles. Volume fraction of the system is defined as $\eta = N\sigma/L$. Because the number N of the particles is small, we should explicitly consider the boundary condition of the system. We will consider two boundary conditions: infinite wall boundary condition (WBC) and periodic boundary condition (PBC).

Let us first consider $\mathrm{N} = 2$ hard spheres under WBC. We can explicitly calculate to obtain

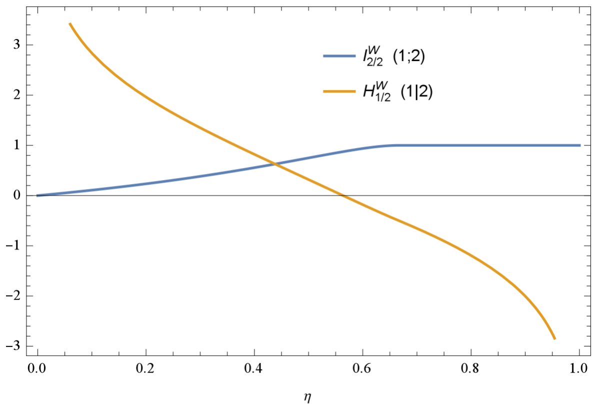
$$I^W_{2/2}(1;2) = \begin{cases} \frac{\eta(4-5\eta)}{4(1-\eta)^2}, & 0 \le \eta < 2/3, \\ 1, & 2/3 \le \eta \le 1, \end{cases}$$

$$H^W_{1/2}(1|2) = \begin{cases} \ln\left(\frac{2}{\eta} - 2\right) - \frac{\eta(4-5\eta)}{8(1-\eta)^2}, & 0 \le \eta < 2/3, \\ -1/2 + \ln\left(\frac{2}{\eta} - 2\right), & 2/3 \le \eta \le 1. \end{cases}$$

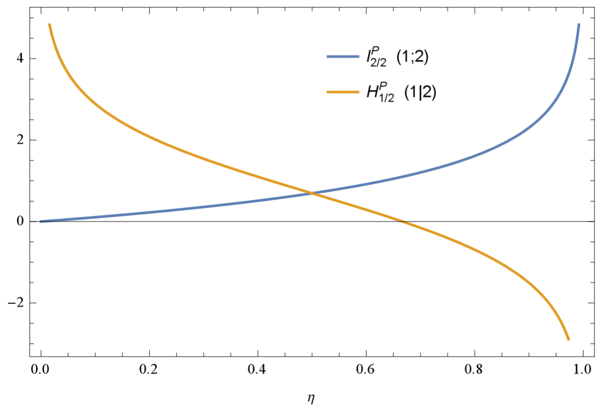
Notice that both $I^W_{2/2}(1;2)$ and $H^W_{1/2}(1|2)$ are piecewise continuous and thus their second order derivatives are discontinuous at $\eta = 2/3$. As shown in Fig. 2a, mutual information $I^W_{2/2}(1;2) \ge 0$ for all the density range $0 \le \eta \le 1$, as it should be. The mutual information $I^W_{2/2}(1;2) = 0$ at $\eta = 0$, implying complete independence, corresponding to an ideal gas system. As the density of the system increases, $I^W_{2/2}(1;2)$ steadily increases up to a value 1 at $\eta = 2/3$ and stays there.

Next, consider N=2 under PBC. The calculated quantities are simply as

$$I^P_{2/2}(1;2) = -\ln(1-\eta),$$

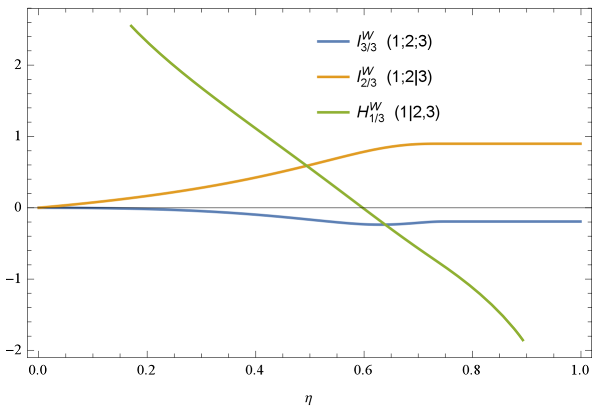


(a) WBC

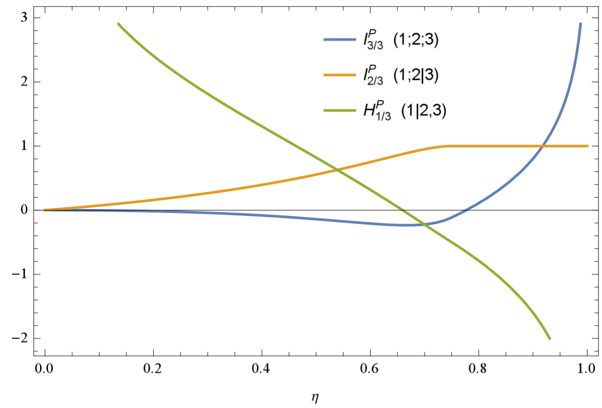


(b) PBC

Fig. 2. (Color online) Decomposed information for N=2 identical particles under hard sphere interaction.



(a) WBC



(b) PBC

Fig. 3. (Color online) Decomposed information for N=3 identical particles under hard sphere interaction.

$$H^P_{1/2}(1|2) = \ln\left(\frac{2}{\eta} - 2\right).$$

Contrary to the WBC case, the curves are continuous everywhere, as shown in Fig. 2b. The mutual information $I^P_{2/2}(1;2)$ steadily increases as the density increases and finally diverges to infinity at $\eta = 1$.

In the case of N=3, mathematical expressions are long and tedious to write down here, thus we omit them. As shown in Fig. 3a, $I^W_{2/3}(1;2|3)$ increases the same as $I^W_{2/2}(1;2)$ and then $I^W_{2/3}(1;2|3)$ becomes less than $I^W_{2/2}(1;2)$ and saturates to a value (2+ln 2)/3 starting from $\eta = 3/4$. $I^W_{3/3}(1;2;3)$ is negative and thus shows a synergy behavior and has a dip with a value -0.236895 at $\eta = 0.629511$ and then stays at a value -0.193147 after $\eta = 3/4$. The fact that $I^W_{3/3}(1;2;3)$ is negative implies that if we know the location of a third particle, then we can predict the locations of the first and the second particles more accurately.

As shown in Fig. 3a, the value $H^W_{1/3}(1|2,3)$ changes sign at $\eta = 0.59735$. As the density of the system increases, the knowledge on particles 2 and 3 enhances the information on particle 1 for $\eta < 0.59735$ and, on the other hand, reduces it for $\eta > 0.59735$. The value $I^W_{2/3}(1;2|3)$ saturates to a value (2+ ln 2)/3 starting from $\eta = 3/4$. The fact that $I^W_{3/3}(1;2;3) < 0$ or $I^W_{2/3}(1;2|3) > I^W_{2/3}(1;2)$ implies that the third one enhances the mutual information between particles 1 and 2. In other words, knowing the position of particle 3 induces an additional correlation, which did not exist between particles 1 and 2.

As shown in Fig. 3b, the value $H^P_{1/3}(1|2,3)$ changes sign at $\eta = 0.659562$. Given the knowledge on particles 2 and 3, the information on particle 1 enhances for $\eta < 0.659562$. At higher density $\eta > 0.659562$, the knowledge, on the other hand, reduces the information on particle 1. The value $I^P_{2/3}(1;2|3)$ saturates to a value 1 from $\eta = 3/4$. The value $I^P_{3/3}(1;2;3)$ has a dip -0.234721 at $\eta = 2/3$ and diverges to infinity at $\eta = 1$. $I^P_{3/3}(1;2;3)$ becomes zero at $\eta = 0.776871$. The fact that $I^P_{3/3}(1;2;3) > 0$ for $\eta > 0.7768711$ implies that the third one, on the other hand, destroys the mutual information between particles 1 and 2. This means that as the density of the system increases there is a transition in triple mutual information from synergy to redundancy.

Comparing between $I^W_{2/3}(1;2|3)$ and $I^P_{2/3}(1;2|3)$, the existence of infinite walls in WBC enhances the mutual information between particles 1 and 2 than PBC case at the same volume fraction in $\eta < 0.651324$, given the information on the position of particle 3. On the other hand, the knowledge on the third increases the mutual information between particles 1 and 2 a little more in PBC than in WBC at higher densities $\eta > 0.651324$.

V. Conclusions

We have formulated statistical mechanics for a thermodynamic system in terms of information theory, which is somewhat different from the Janes's maximal entropy method [12]. Interaction between particles in the system induces mutual information on positions between two or more particles. Thus, the interaction between the constituent particles can be interpreted as an exchange of spatial information in the system. We can thus analyze the thermodynamical system using information contents contained in the system. The existence of the boundary affects the mutual information of the system. We have explicitly calculated triple mutual information for hard sphere systems in WBC and PBC. For N=3 system, as the density of the system increases, there is a transition in triple mutual information from synergy to redundancy under PBC. This behavior may be deeply connected with the jamming behaviors and also give some insight for understanding why the problem of the triangular relationship is so difficult to resolve.

Mutual information change occurs internally due to interaction between particles and external control of thermodynamic states and boundary conditions. This formulation can be very effective in analyzing a small thermodynamic system. As the thermodynamic variables change, the mutual information between particles accordingly change. The system may react to adapt these changes of mutual information. In this way, the biological systems may use or adapt itself in accordance of mutual information transferred from other particles or systems. Therefore, this formalism can be readily used to analyze the biological systems. We can thus obtain a different understanding of the physical/chemical/biological behaviors of the system in another perspective [8].

Our consideration in one-dimensional space is rather simple and easy. Generalization to a higher dimensional space may not be impossible but becomes rather difficult. If we extend to higher dimensions, we should take into account of distance measure and various boundary conditions for the system. Also, generalization to a quantum system may be rather straightforward if we adopt density matrix and quantum information formalism. We can also readily extend this formulation to more complex potential models, or larger particle number systems by employing numerical methods. The formalism developed in this article can be used in analyzing or explaining many-body problems in theory or in simulation and can be experimentally tested by employing nanotechnology.

ACKNOWLEDGEMENTS

This work was supported by 2018 Research Grant of Kyonggi University.

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