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A Connection for a Partially Asymmetric Driven Lattice Gas of a Mean-Field Type to an Exact Lattice Density Functional Via a Diagrammatic Method

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Abstract. A relationship of the totally asymmetric simple exclusion process (TASEP) of particles on a one-dimensional lattice system that interact with site exclusion to an exact density functional has been established in [1]. Here, the connection is extended for a partially asymmetric exclusion process (PASEP) where particles on a one-dimensional lattice system may be driven to the left or to the right with certain (left and right) hopping rates. The mean-field equation for the one-particle density of the PASEP is equivalent to the exact equilibrium density of a lattice fluids mixture with three species. The connection is put forward by associating the particles in the lattice fluids mixture to the particle and the particle movements in the PASEP. The particle densities of the lattice fluids mixture is obtained based on the lattice fundamental measure theory via a diagrammatic method. Omitting one of the particles in the mixture yields back the relationship given in [1].

Keywords: PASEP, hopping rates, lattice fluids mixture.
PACS: 05

INTRODUCTION

Exclusion processes are a class of driven diffusive systems which are widely used to model non-equilibrium phenomena such as transport processes in biological systems [2,3], bio-polymerization [4,5], vehicular traffics [6-11], and performance of wireless network [12]. This model consists of hard-core particles moving (jumping) through a one-dimensional lattice sites with certain dynamical rule and boundary conditions. In this paper in particular, the model being studied is the partially asymmetric simple exclusion process (PASEP). Here, particles may move to the right (left) nearest neighbor site with hopping rate k_+ (k_-). If one of the hopping rate is set to zero, e.g. $k_- = 0$, then the well known totally asymmetric simple exclusion process (TASEP) [13, 14] is obtained.

A relationship based on a mean-field theory between the TASEP and the equilibrium lattice gas through classical density functional theory is given in [1]. This relationship is obtained by a correspondence between the appropriate particles of the binary mixture to the resting and moving particles of the TASEP. It is demonstrated in [1] that the mean-field equation of motion for the one-particle density of the TASEP is equivalent to the exact Euler-Lagrange equations for the equilibrium density profiles of a binary mixture. Especially in this article, the aforementioned connection is to be applied for the PASEP. To our knowledge this relationship has not been published.

Classical density functional theory (DFT) [15, 16] is a powerful tool based on a variational principle which has become a standard framework to study static physical properties of equilibrium systems. The theory is applied to study various phenomena in inhomogeneous fluids, such as freezing and surface and interface behavior [17]. Classical DFT is recently used to treat aromatic ionic liquids at room temperature [18] and hydration of complex surfaces [19]. In principle, the aim of classical DFT is to construct an (approximate) free energy functional F of a classical system. Moreover, F can be written as a functional of the one-body density, $\rho(\mathbf{r})$, that is $F[\rho(\mathbf{r})]$, where $\mathbf{r}$ is the position of an averaged number of particles. $F[\rho(\mathbf{r})]$ may eventually be determined via the Legendre transform of the grand potential, $\Omega[\rho(\mathbf{r})]$, which is also a functional of $\rho(\mathbf{r})$. Functional derivate of $F[\rho(\mathbf{r})]$ produces the one-body

direction correlation function, viz. $c^{(1)}$. Finally, minimizing $\Omega[\rho(\mathbf{r})]$ with respect to $\rho(\mathbf{r})$ yields the true one-body density at equilibrium. In this article, a method of classical DFT for hard core lattice models is utilized, i.e. the lattice fundamental measure theory (LFMT). LFMT is initially proposed in [20-22] as an extension of the FMT [23], which is developed based upon the molecular volume and other fundamental geometric measures of individual molecules [24].

THE FREE ENERGY FUNCTIONAL

The free energy functional only depends upon the interaction of the constituents of the system. The quantity is conveniently split into two parts, which is the ideal and the excess over ideal free energies, i.e.: F_{id} and F_{ex}, respectively. For lattice systems the excess free energy functional in one-dimension (1D) may be defined as

$$F_{\text{ex}}\left[\rho_{i=1}(x),\ldots\rho_N(x)\right]\equiv F\left[\rho_1(x),\ldots\rho_N(x)\right]-F_{\text{id}}\left[\rho_1(x),\ldots\rho_N(x)\right], \quad (1)$$

where $i = 1,\ldots,N$ denotes the species present in the system and $\rho_i(x)$ is the density of species i at lattice site x. The ideal free energy functional for lattice systems may be expressed as

$$F_{\text{id}}=\frac{1}{\beta}\sum_{i=1}^{N}\sum_{x\in S}\rho_i(x)\left[\ln\left(\rho_i(x)\right)-1\right], \quad (2)$$

with $1/\beta = k_BT$, k_B is the Boltzmann constant, T is the temperature, and S is the lattice system. The excess free energy functional for any 1D hard-core lattice fluids is

$$F_{ex}[\rho]=\frac{1}{\beta}\sum_{x\in S}\sum_{k\in I}a_k\Phi_0\left(n^{(k)}(x)\right), \quad (3)$$

where I is the set of indices suitably chosen to label every weighted densities $n^{(k)}(x)$, Φ_0 is the excess free energy of the 0D cavity [25], and a_k is the integer coefficient of Φ_0. The weighted density $n^{(k)}(x)$ may be defined as

$$n^{(k)}(x)\equiv\sum_{i=1}^{N}\sum_{t\in C_{i,0D}^{(k)}(x)}\rho_i(t), \quad (4)$$

where $C_{i,0D}^{(k)}$ is the k-th subset of $x \in S$, which is the appropriate 0D cavity of species i. Finally, the excess free energy functional for any 0D cavity in 1D is given by

$$\Phi_0(\eta)=(1-\eta)\ln(1-\eta)+\eta, \quad (5)$$

with $0 \le \eta \le 1$ is the averaged number of particles in the 0D cavity.

It may be observed that the ideal free energy functional is already provided by equation (2). However, the excess free energy functional is still unknown and depends upon the system under consideration. There is currently three methods to approximate functional (3), that is i) algebraic method, ii) diagrammatic method, and iii) Mobius inversion method. Here, the diagrammatic method is demonstrated. But before the method is used, as mentioned above, the models under consideration and their relationship have to be explained.

THE MODELS AND THEIR RELATIONSHIP

The dynamical model studied is the PASEP. This model consists of discrete lattice sites, S, and hard-core particles occupying the lattice sites. At each time steps, a site, $x \in S$, is chosen randomly with probability $1/N$. If there is a particle on the chosen site, the particle may jump to the right (left)-nearest neighbor site with hopping rate k_+ (k_-) provided that there is no particle occupying the right (left)-nearest neighbor site. This is illustrated in Fig. 1.

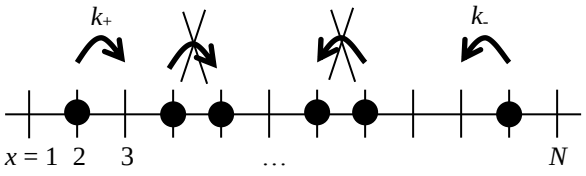


FIGURE 1. The PASEP in 1D. The lattice sites are the vertical lines denoted by x = 1, 2, 3,…, N. The big dark dots are the hard-core particles. The arrows show the movement of particles. The crosses show that the particles are not allowed to jump.

From the model above, the averaged quantities which we are interested in are the current density of particles moving to the right (left) and the density of particles occupying the sites, i.e.: $j_+(x)$ [$j_-(x)$] and $\rho(x)$, respectively. These quantities describe the macroscopic behavior of the PASEP. According to [1], the aforementioned quantities may be obtained via a connection to the appropriate equilibrium lattice fluids mixture. This connection is given as follows. A particle that jumps to the right (left)-nearest neighbor site (see Fig. 1) corresponds to a dimer that has site exclusion and excludes its right (left)-nearest neighbor site (see Fig. 2), i.e. denoted by L_1 and L_2, respectively. A particle that does not jump (stays at the site) corresponds to a monomer (L_3) that only excludes its own site.

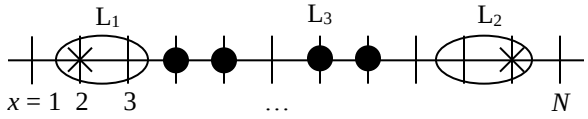
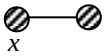


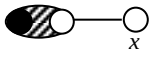
FIGURE 2. The equilibrium hard-core lattice fluids mixture with three species. L_1 and L_2 are dimers with positions at $x = 2$ and $x = N - 1$, respectively. L_3 is a monomer.

From the correspondence above, the lattice fluids mixture with three species is obtained (Fig. 2). In this system, the averaged quantities are the densities of L_1, L_2, and L_3, viz.: $\rho_{L1}(x)$, $\rho_{L2}(x)$, and $\rho_{L3}(x)$, respectively. These three quantities are the Euler-Lagrange equations obtained later from the LFMT. Following the correspondence above, the relationship between the averaged quantities of the lattice fluids mixture and the PASEP is provided as follows. The densities of the dimers, i.e.: $\rho_{L1}(x)$ and $\rho_{L2}(x)$, may be realized as the density currents, i.e.: $j_+(x)$ and $j_-(x)$, respectively, whereas the monomer, $\rho_{L3}(x)$, may be realized as the density of the particles of the PASEP, $\rho(x)$. Hence, the task now is to determine $\rho_{L1}(x)$, $\rho_{L2}(x)$, and $\rho_{L3}(x)$ through the diagrammatic method of LFMT, such that $j_+(x)$, $j_-(x)$, and $\rho(x)$ may be finally gained.

F_{ex} CALCULATION VIA THE DIAGRAMMATIC METHOD

Before we determine the Euler-Lagrange equations, the F_{ex} has to be calculated in advance. Construction of the F_{ex} begins by determining the maximal cavities [25] of the species, i.e.  ,  , and  for L_1, L_2, and L_3, respectively.

The circles represent the lattice sites where the position of the particles is denoted by x. Hence, the maximal cavities of the mixture are

 and  .

It may be observed that the maximal cavities above are the combination of the maximal cavities of the species. Hence, the first guess of the F_{ex} in accordance with equation (3) is attained as

$$\beta F_{\text{ex}} = \sum_{x\in S}\Big[\Phi_0\Big(\quad\Big) + \Phi_0\Big(\quad\Big)\Big]. \tag{6}$$

The functional (6) needs to be evaluated using any density profile, e.g.:  as a test for the 0D density profile. The evaluation produces spurious terms that have to be eliminated. This is done by introducing a second guess for the F_{ex}, i.e.:

$$\beta F_{\text{ex}} = \sum_{x\in S}\Big[\Phi_0\Big(\quad\Big) + \Phi_0\Big(\quad\Big)\Big] + \sum_{x\in S}\Phi_0\Big(\quad\Big). \tag{7}$$

Using the same 0D density profile as a test for functional (7), yields the correct F_{ex} , that is

$$\beta F_{ex} = \sum_{x\in S}\Big[\Phi_0\Big(\quad\Big) + \Phi_0\Big(\quad\Big)\Big] + \sum_{x\in S}\Big[\Phi_0\Big(\quad\Big) + \Phi_0\Big(\quad\Big)\Big]. \tag{8}$$

Moreover, since every cavity is associated to its density function, then we have from functional (8),

$$\begin{aligned}\beta F_{\text{ex}} = \sum_{x\in S}\Big\{&\Phi_0\big[\rho_{L_1}(x)+\rho_{L_1}(x+1)+\rho_{L_2}(x)+\rho_{L_3}(x)\big]\\ &+\Phi_0\big[\rho_{L_1}(x-1)+\rho_{L_2}(x-1)+\rho_{L_2}(x)+\rho_{L_3}(x)\big]\\ &-\Phi_0\big[\rho_{L_1}(x)+\rho_{L_2}(x+1)\big]-\Phi_0\big[\rho_{L_1}(x)+\rho_{L_2}(x)+\rho_{L_3}(x)\big]\Big\},\end{aligned} \tag{9}$$

with each of the excess free energy of the 0D cavity, Φ, satisfies equation (5). Functional (9) is the exact excess free energy for the lattice fluids mixture with three species.

THE EULER-LAGRANGE EQUATIONS

The Euler-Lagrange equations can be determined using equations (1), (2), and (9). By calculating the direct correlation function for each species i, i.e.:

$$c^{(1)}_{\rho_i} = -\frac{\partial \beta F_{ex}}{\partial \rho_i(x')}, \tag{10}$$

then setting low densities of the dimers, that is, ρ_{L1}, $\rho_{L2} \to 0$, and finally inserting the results into the Euler-Lagrange equation, viz.:

$$\rho_i(x) = e^{c^{(1)}_{\rho_i}} e^{\beta V_i(x)}, \tag{11}$$

where V_i is any external potential acting upon species i, produces:

$$\rho_{L_1}(x) = e^{\beta\left|V_{L_1}(x)-V_{L_3}(x)\right|}\rho_{L_3}(x)\big[1-\rho_{L_3}(x+1)\big], \tag{12}$$

$$\rho_{L_2}(x) = e^{\beta\left|V_{L_2}(x)-V_{L_3}(x)\right|}\rho_{L_3}(x)\big[1-\rho_{L_3}(x-1)\big], \tag{13}$$

and

$$\rho_{L_3}(x) = e^{V_{L_3}(x)}\big(1-\rho_{L_3}(x)\big). \tag{14}$$

Equations (12) – (14) are in fact the density profiles of the species in the equilibrium lattice fluids mixture system.

THE DENSITY AND CURRENT DENSITY OF THE PASEP

Finally, the macroscopic description of the PASEP, especially its one-particle and current densities may be achieved using equations (12) – (13). Invoking again the relationship given in the previous part, that is $j_+(x) \rightarrow \rho_{L1}(x)$, $j_-(x) \rightarrow \rho_{L2}(x)$, and $\rho(x) \rightarrow \rho_{L3}(x)$, and also introducing two more relationships, $e^{\beta[V_{L_1}(x)-V_{L_3}(x)]} \rightarrow k_+(x)$ and $e^{\beta[V_{L_2}(x)-V_{L_3}(x)]} \rightarrow k_-(x)$, produces

$$j_+(x) = k_+(x)\rho(x)[1-\rho(x+1)], \quad (15)$$

and

$$j_-(x) = k_-(x)\rho(x)[1-\rho(x-1)]. \quad (16)$$

In addition, the density of the PASEP may be acquired by bringing into play the continuity equation,

$$\left.\frac{\partial\rho(x,t)}{\partial t}\right|_{\text{tot}} = -(\nabla j_+ + \nabla j_-), \quad (17)$$

with $\nabla j_+(x) \equiv j_+(x\text{-}1) - j_+(x)$ and $\nabla j_-(x) \equiv j_-(x\text{+}1) - j_-(x)$. In steady state, the LHS of equation (17) goes to zero, which then produces

$$\rho(x) = \frac{\{k_+\rho(x-1)[1-\rho(x)] + k_-\rho(x+1)[1-\rho(x)]\}}{k_+[1-\rho(x+1)] + k_-[1-\rho(x-1)]}, \quad (18)$$

which is just the density of the PASEP at steady state. It may be observed that equations (15), (16), and (18) are essentially mean-field equations. They are not the exact solution for the PASEP. However, the Euler-Langrange equations of the lattice fluids mixture are exact. Equation (17) is not a closed equation but may easily be solved self-consistently using numerical methods. It may also be noticed that setting one of the hopping rate to zero, e.g. $k_-(x) = 0$ in (16) yields back the known TASEP model.

CONCLUSION

The relationship between the PASEP and the lattice fluids mixtures has been presented. The relationship is based upon a correspondence between the particles and the jumping of particles of the PASEP with the species of the lattice fluids mixture. The (excess) free energy functional is calculated using the LFMT via a diagrammatic method, such that the Euler-Lagrange equations are obtained. Hence, the density and current densities of the PASEP are achieved by invoking the aforementioned relationship.

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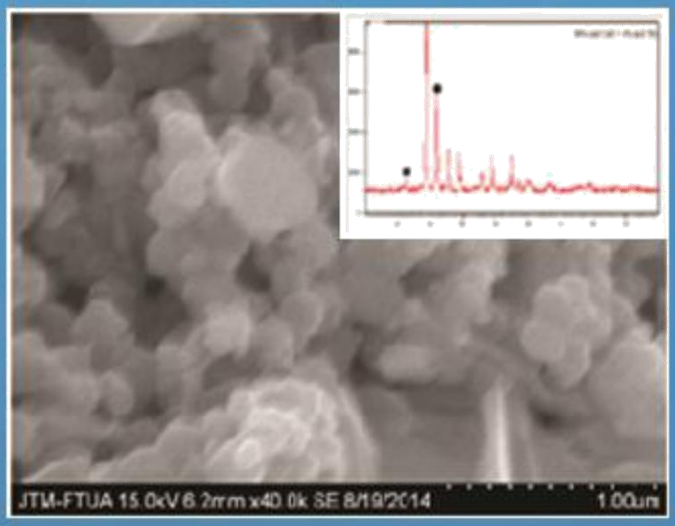

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PREFACE

The *4th International Conference on Theoretical and Applied Physics* (*ICTAP*) 2014 was held in Bali, Indonesia on October 16-17, 2014. It is an international conference covering a wide subject in the field of theoretical and applied physics. This Conference was organized by the Department of Physics, Udayana University (UNUD) and Indonesian Physical Society (HFI). Many people have unreservedly and enthusiastically participated in the planning and preparation of this conference, including the Organizing and Scientific Committees, the speakers, the conference officer, students, etc. Thank you all for your positive attitude and fantastic support. Thanks to all invited speakers: Prof. Dr. Yusaku Fujii (Gunma University, Japan), Prof. Jakrapong Kaewkhao, Ph.D (Nakhon Pathom Rajabhat University, Thailand), Prof. Dr. Hong Joo Kim (Kyungpook National University, Republic of Korea) and Prof. Dr. Ing Mitra Djamal (ITB) that you have accepted our invitation. The financial support from Udayana University is gratefully acknowledged. ICTAP 2014 is aimed at providing the much needed forum of scientific communication and interaction among distinguished scientists working in the field of physics and related fields.

This event was also designed to offer the opportunity of making direct contact for the young Indonesian scientists and students with well-known scientists abroad and thereby fostering the existing research collaborations and extending international research networking for the future.

More than 106 authors from 6 countries have submitted their work in the conference. ICTAP 2014 finally accepted 57 original research papers after a peer review process. During the conference, 14 parallel sessions were held in order to advance and contribute to specific research area in physics.

Finally, special thanks to you, the delegates, for supplying the input needed for successful scientific conferences. We wholeheartedly welcome you and hope you find ICTAP 2014 as successful and rewarding as we envision it to be.

Denpasar, 12 May 2016

Editors

Ni Nyoman Rupiasih, Ph.D.
Dr. Wayan Gede Suharta
Dr. Hery Suyanto

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