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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], biopolymerization [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

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

where $i = 1, \dots, N$ 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

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

with $1/\beta = k_B T$, 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

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

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 $0 \leq \eta \leq 1$ 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.

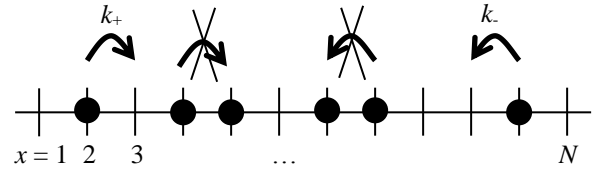


FIGURE 1. The PASEP in 1D. The lattice sites are the vertical lines denoted by $x = 1, 2, 3, \dots, N$. The big dark dots are the hard-core particles. The arrows show the movement of particles. The crosses show that the particles are not allowed to jump.

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.

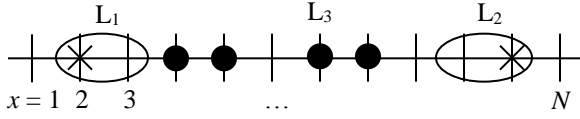
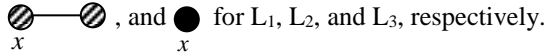


FIGURE 2. The equilibrium hard-core lattice fluids mixture with three species. L_1 and L_2 are dimers with positions at $x = 2$ and $x = N - 1$, respectively. L_3 is a monomer.

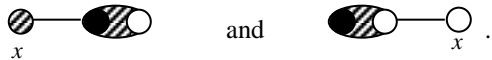
From the correspondence above, the lattice fluids mixture with three species is obtained (Fig. 2). In this system, the averaged quantities are the densities of L_1 , L_2 , and L_3 , viz.: $\rho_{L_1}(x)$, $\rho_{L_2}(x)$, and $\rho_{L_3}(x)$, respectively. These three quantities are the Euler-Lagrange 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.: $\rho_{L_1}(x)$ and $\rho_{L_2}(x)$, may be realized as the density currents, i.e.: $j_+(x)$ and $j_-(x)$, respectively, whereas the monomer, $\rho_{L_3}(x)$, may be realized as the density of the particles of the PASEP, $\rho(x)$. Hence, the task now is to determine $\rho_{L_1}(x)$, $\rho_{L_2}(x)$, and $\rho_{L_3}(x)$ 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. $\bigcirc - \bigcirc$,



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



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

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

The functional (6) needs to be evaluated using any density profile, e.g.: $\textcircled{\text{---}}\textcircled{\text{---}}$ 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.:

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

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

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

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

$$\beta F_{ex} = \sum_{x \in S} \{ \Phi_0[\rho_{L_1}(x) + \rho_{L_1}(x+1) + \rho_{L_2}(x) + \rho_{L_3}(x)] + \Phi_0[\rho_{L_1}(x-1) + \rho_{L_2}(x-1) + \rho_{L_2}(x) + \rho_{L_3}(x)] - \Phi_0[\rho_{L_1}(x) + \rho_{L_2}(x+1)] - \Phi_0[\rho_{L_1}(x) + \rho_{L_2}(x) + \rho_{L_3}(x)] \}, \quad (9)$$

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.:

$$c_{\rho_i}^{(i)} = - \frac{\partial \beta F_{ex}}{\partial \rho_i(x')}, \quad (10)$$

then setting low densities of the dimers, that is, $\rho_{L_1}, \rho_{L_2} \rightarrow 0$, and finally inserting the results into the Euler-Lagrange equation, viz.:

$$\rho_i(x) = e^{c_{\rho_i}^{(i)}} e^{\beta V_i(x)}, \quad (11)$$

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

$$\rho_{L_1}(x) = e^{\beta[V_{L_1}(x) - V_{L_3}(x)]} \rho_{L_3}(x) [1 - \rho_{L_3}(x+1)], \quad (12)$$

$$\rho_{L_2}(x) = e^{\beta[V_{L_2}(x) - V_{L_3}(x)]} \rho_{L_3}(x) [1 - \rho_{L_3}(x-1)], \quad (13)$$

and

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

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, $e^{\beta[V_{L1}(x)-V_{L3}(x)]} \rightarrow k_+(x)$ and $e^{\beta[V_{L2}(x)-V_{L3}(x)]} \rightarrow k_-(x)$, 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 $\nabla j_+(x) \equiv j_+(x-1) - j_+(x)$ and $\nabla j_-(x) \equiv j_-(x+1) - j_-(x)$. 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-Lagrange 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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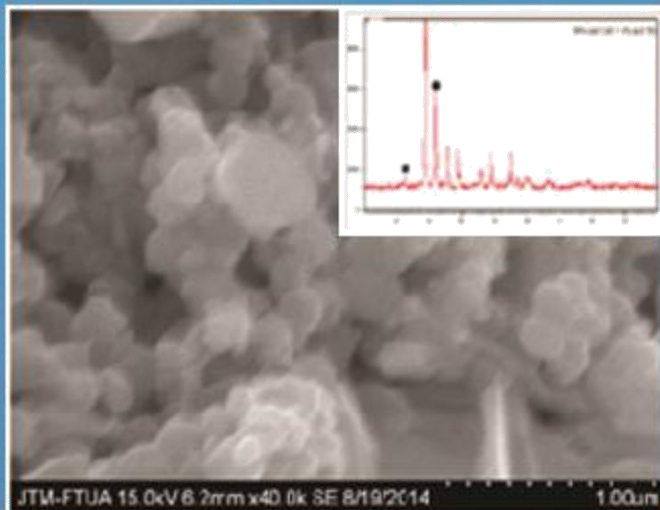
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**Bali, Indonesia
16 - 17 October 2014**



Editors :

**Ni Nyoman Rupiasih, Wayan Gede Suharta and Hery Suyanto
Udayana University, Bali, Indonesia**

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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

Table of Contents

	PLENARY AND INVITED PAPERS	page
KS-1	Review of the Levitation Mass Method (LMM) – A Precision Method for Measuring Mechanical Quantities Using An Optical Interferometer, <i>Yusaku Fujii, Hadi Nasbey, Agus Setyobudi and Akihiro Takita</i>	001-006
KS-2	White Emission Materials from Glass Doped with Rare Earth Ions, <i>P. Yasaka and J. Kaewkhao</i>	007-020
	Parallel Session TC: Theoretical Physics and Computation	
TC 1-01	Application of quantum heat engine on the three-dimensional potential, <i>Andika Kusuma Wijaya</i>	021-026
TC 1-05	Direct Method of Calculus of Variation on Electromagnetism in Differential Form, <i>I Gusti Ngurah Yudi Handayana and Muhammad Farchani Rosyid</i>	027-034
TC 1-07	Chaos Identification of the Double Pendulum Motion in the Magnetic Field by <i>Joko Saefan and Suparmi</i>	035-040
TC 1-10	Computer Simulation Development base on Open Source to improve Students Conceptual Competence, <i>Madlazim and Dyah Permatasari</i>	041-050
TC 1-15	Quantum Physics Learning by Using Matlab 7.6 on Highlights Potential Transmission Coefficient Parabolic One Dimension, <i>Reni Herniati and Andika Kusuma Wijaya</i>	051-055
TC 1-21	A Connection for a Partially Asymmetric Driven Lattice Gas of A Mean-Field Type to an Exact Lattice Density Functional Via a Diagrammatic Method, <i>Wipsar Sunu Brams Dwandaru and Matthias Schmidt</i>	056-061
TC 1-23	Theoretical EQUATION WITH EVIDENCE Relaxation oscillator using an oscilloscope ON THE CIRCUITS OP-AMP, <i>Yohanes Soenarto, Imas Ratna Ermawaty, Tri Isti Hartini and Felicianda</i>	062-069
	Parallel Session AM: Advanced Material and Nanotechnology	
AM 1-02	LPG Gas Sensing Properties of Composite CuO(TiO ₂) Sensor, <i>Elvaswer, Muhammad Faisal, Dwi Puryanti, Essy Puspa Zelvya and Ratna Sari Dewi</i>	070-073
AM 1-04	Electrodeposition and Characterization of Ni-TiAlN Composite Film, <i>Esmar Budi, Agus Setyo Budi, Iwan Sugihartono, Setia Budi and Hadi Nasbey</i>	074-079
AM 1-06	Effect of Cold Isostatic Pressing on Properties of Millimeter Wave Sintered High Purity Alumina, <i>Ida Usman, I Nyoman Suidiana, La Ode Ngkoimani and Usman Rianse</i>	080-083
AM 1-07	The Preparation of Natural Rubber –g-Glycidil Metacrilate Nanocomposite, <i>Kurnia Sembiring and Riani Sari Sembiring</i>	084-092
AM 1-29	Characterization Of ZnO Thin Films Doped with Natrium by Sol-Gel Method, <i>P.L. Gareso, N. Syuhada, N. Rauf, E. Juarlin, Sugianto and A. Maddu</i>	093-097

AM 1-30	The Influence of the Milling Time Process on Microstructure and Magnetic Properties of Isotropic Bonded NdFeB Magnets, <i>Priyo Sardjono, Muljadi, Nenen Rusnaeni, Suprapedi and Ayu Yuswitasari</i>	098-102
Parallel Session BM: Biophysics and Medical Physics		
BM 1-01	Concentrations of Some Natural Occurring Radionuclides and Particles during the 2010 Eruption of Mount Bromo in East Java, Indonesia, <i>Johan A.E. Noor</i>	103-106
BM 1-02	Automatic thresholding with Otsu Method To Identify Plasmodium falciparum Phase in Malaria-infected Red Blood Cells, <i>Kusworo Adi, Sri Pujiyanto, Rahmat Gernowo, Adi Pamungkas and Ari Bawono Putranto</i>	107-112
BM 1-04	Head Impact Analysis of Children in Soccer Heading, <i>Nugroho Agung S., Tommy Apriantono and Suprijanto</i>	113-117
BM 1-06	Development of Low-Cost Modular Wireless EEG System, <i>Andri Rahmadhani, Sra H. Pratama, Suprijadi, Freddy Haryanto and Suparno Satira</i>	118-122
BM 1-08	Analyzis of Computed Tomography Dose Index (CTDI) value towards X-ray Tube Current and Voltage Variations of Computed Tomography Scanner (CT Scan) by using PPMA Phantom, <i>Syamsir Dewang, Bualkar Abdullah, Bannu, Nur Hasanah, Suryaningsih and Satrial Male</i>	123-127
BM 1-11	Burnable Poison Neutronic Characteristics of Hexagonal Tight Lattice Cell for Small Long-Life BWR with Thorium Based Fuel, <i>Nuri Trianti, Zaki Su'ud, Idam Arif, Sidik Permana and Eka Sapta Riyana</i>	128-134
Parallel Session G: Geophysics		
G 1-01	Estimation of Ore Body Distribution at X-Field, Nangroe Aceh Darussalam Province, Using Resistivity Method, Dipole-Dipole Configuration, <i>Adi Susilo</i>	135-139
G 1-02	Estimating Reservoir Temperature Using Geothermometer Equation On Hot Springs In Panti District, Pasaman Regency, West Sumatera, Indonesia, <i>Ardian Putra and Rahmat Arrahman</i>	140-143
G 1-03	Relation Model between Electrical and Mechanical Properties on the Exploration Sub Surface under Ground, <i>Lantu1, D.A. Suriamihardja, A.M. Imran and Tri Harianto</i>	144-147
G 1-04	The Geothermal Model of Dieng Plateau Complex from Resistivity Image With Magnetotelluric Method, <i>Eddy Z Gaffar</i>	148-153
G 1-07	Application of Geoelectrical Resistivity Method to Investigate Subsurface Geology Structure of Lava Spill Area of Gamalama Volcano, <i>Fatma Hamid, Saprudin, M. Toifur and Yudhiakto Pramudya</i>	154-159
G 1-08	Analysis Of Subsurface Materials Based On The Price Of Medium Permeability In The Karst Region Pangkep, <i>Muhammad Arsyad, Nasrul Ihsan and Vistarani Arini Tiwow</i>	160-164
G 1-17	The Analysis of P-Wave Period-Duration as One of Parameters for Tsunami Early Warning, <i>Zulkarnain Adnan, Sugeng Pribadi and Nanang T. Puspito</i>	165-170
G 1-18	Specific Solutions Groundwater Flow Equation, <i>Muhammad Hamzah Syahrudin</i>	171-174

	Parallel Session A: Astrophysics	
A 1-01	Study of Ideal Magnetohydrodynamics In Curved Space, <i>Luh Putu Budi Yasmini, and I Gede Aris Gunadi</i>	175-178
	Parallel Session IP: Instrumental Physics	
IP 1-01	Development of Web-based Power Monitoring System for a Pulse Combustion Spray Pyrolysis using Java Programming, <i>Agus Fatrya Nanda, Darmawan Hidayat, Camellia Panatarani, Dwindra W. Maulana and I Made Joni</i>	179-183
IP 1-03	Digital Receiver Synchronization Methods for OFDM Modem, <i>Assa'idah and Hadi</i>	184-189
	Parallel Session LO: Laser and Opto-electronics	
LO 1-02	Dependence of the defect modes on the strength of localized defects in photonic lattice, <i>Arif Hidayat, Diana Kurniati, Hari Wisodo and Eny Latifah</i>	190-197
LO 1-05	Potential Candidate for Gigahertz range Electromagnetic wave absorbers of Carbon Sheets Based on Polymer, <i>Maria Margaretha Suliyanti, Nanik Indayaningsih and Affi Nurhidayah</i>	198-203
LO 1-08	Study on the Theory of Electron Multiple Scattering on Plasma, <i>Taat Guswantoro, Muhammad Nur and Vincencius Gunawan</i>	204-209
	Parallel Session EE: Energy and Environment Physics	
EE 1-03	Development Of Wind Tunnel For Aerodynamic Test To Support The Wind Energy Research, <i>Hadi Nasbey , Cecep Rustana and Christine Steffhanie</i>	210-215
	Parallel Session I: Interdisciplinary Physics	
I 1-01	A Misunderstanding of Force Concept; the action-reaction pairs same as a cause-effect sequence, <i>A. Halim, Melvina and Susilawati</i>	216-219
I 1-04	A Study on The Physical Characteristics of Lemukutan Island Territorial Water Wave in Bengkayang Regency, <i>Eka Murdani and Sumarli</i>	220-224
I 1-08	The Influence of Cooperative Instructional Strategies with STAD Technique on Students Achievement in Physics of Grade XI SMA Lab School, Palu, <i>Marungkil Pasaribu</i>	225-229
I 1-11	The Relationship between Formal Thinking Abilities and Problem-Solving Skills in Kinematics Topics, <i>Sondang R. Manurung</i>	230-234
I 1-12	Theoretical Modeling for the Effect Tenacity on Take-Up Roller (Ro) and Tenacity on Winding Device (Rw) Related With the Yarn Breakage on Rotor Open End Spinning, <i>Valentinus Galih Vidia Putra, M.F. Rosyid and R. Arief Dewanto</i>	235-240
I 1-14	Comparative Study of Gas Chromatography-Mass Spectrometry in FAME and FAEE of Virgin Coconut Oil, <i>Ni Made Suaniti and I Wayan Bandem Adnyana</i>	241-245