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<td>14:20-14:50</td>
<td>Ms. Pei-Yin Chi (Nano Science and Technology, Taiwan International Graduate Program, Academia Sinica)</td>
<td>Characterizing nucleus deformation of cancer cells through microfluidic slit orifice</td>
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<td>14:50-15:20</td>
<td>Mr. Guan-Rong Huang (Department of Physics, National Taiwan University)</td>
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<td>15:40-16:10</td>
<td>Mr. Xuhui Xiao (Department of Physics, National Taiwan University)</td>
<td>A simplified lattice model for polypeptide fibril transitions</td>
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<td>16:10-16:40</td>
<td>Ms. Yu-Hsin Hsieh (Department of Physics, National Taiwan University)</td>
<td>Heat capacity components carried by partition function zeros in interacting self-avoiding walks</td>
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Organizers: National Center for Theoretical Sciences (Critical Phenomena and Complex Systems focus group) and Institute of Physics of Academia Sinica (Taipei)
Website: http://proj1.sinica.edu.tw/~statphys/
Abstract

Dr. Jengjan Tsai (Institute of Physics, National Chiao Tung University; E-mail: jengjian@gmail.com)

Talk Title: Tracer Particle Response Mapped to Microorganism-flagellum-rotor Matrix Behavior

Abstract: Inspired by the scientific curiosity and the possible reality application about the microorganism-flagellum action behavior. Two minimal models, microorganism-flagellum-rotor (MFR) model (equivalent to MFRmatrix model) and microorganism-flagellum-rotor sweep (MFRsweep) model are proposed to mimic the so complex microorganism flagellum rotation and sweep behaviors in real world. By utilizing these two minimal models the hydrodynamic interaction phenomena, take both of the completeness Blake-Oseen tensor (BOT) $G^c$ and the approximation Blake-Oseen tensor $G^s$ into account, are exploited in the following issues: (1) 2 MFRs (2) an $N \times N$ MFRs constituted matrix (3) a tracer particle located over an $N \times N$ MFRs constituted matrix are explored. A phase diagram is discovered in issue (1). The synchronization state existence condition, and the repellency and freezing states existence conditions are studied in issue (2). A circular motion (CM) mode, a linear oscillation (LO) mode, and a sharp jumping (SJ) mode are researched in issue (3). Some recent experimental outcomes that related to the bacterial carpet action can be explained reasonably from MFRmatrix and MFRsweep models.

References:

Mr. Hsin-Lin Chiang (Department of Physics, National Tsing-Hua University; E-mail: jiangsl@phys.sinica.edu.tw)

Talk Title: Oligomerization of peptides LVEALYL and RGFFYT and their binding affinity to insulin

Abstract: Recently it has been proposed a model for fibrils of human insulin in which the fibril growth proceeds via stacking LVEALYL(fragment 11-17 from chain B of insulin) into pairs of tightly interdigitated β-sheets. The experiments have also shown that LVEALYL has high propensity to self-assembly and binding to insulin. This necessitates study of oligomerization of LVEALYL and its binding affinity to full-length insulin. Using the all-atom simulations with Gromos96 43a1 force field and explicit water it is shown that LVEALYL can aggregate. Theoretical estimation of the binding free energy of LVEALYL to insulin by the molecular mechanic Poisson-Boltzmann surface area method reveals its strong binding affinity to chain B, implying that, in agreement with the experiments, LVEALYL can interfere with insulin aggregation via binding mechanism. We predict that, similar to LVEALYL, peptide RGFFYT (fragment B22-27) can self-assemble and bind to insulin modulating its fibril growth process. The binding affinity of RGFFYT is shown to be comparable with that of LVEALYL.

Dr. Shih-Chieh Wang (Institute of Physics, Academia Sinica; E-mail: scwang1979@gmail.com)

Talk Title: The stock price mean-square-log-return study of the US and Taiwan stock markets

Abstract: This talk introduces our recent discovery [Ma et,al., EPL 102,66003 (2013)] that the time dependence of mean-square log-return $\left\langle \xi^2(t) \right\rangle$ calculated from one-day-moving-averages(1DMA) of stock prices in the US and Taiwan stock market over range $\tau = 36 \sim 1.08 \times 10^5$ seconds is analogous to that of the mean square displacement of ballistic Langevin particles in a hydrodynamic system. From such an analogy, we are able to obtain a master curve by fitting data of collections of 345 stocks...
for each market, that temperature-like and diffusivity-like kinetic parameters jointly serve as scale-readjustment factors over the two asymptotic regimes, of exponents 2.0 and 1.0, respectively.

Mr. Kuo-Ting Tsai (Department of Physics, National Kaohsiung Normal University; E-mail: kuoting.tsai@gmail.com)
Talk Title: Phase locking route behind complex periodic windows in a forced oscillator
Abstract: Chaotic systems have complex reactions against an external driving force; even in cases with low-dimension oscillators, the routes to synchronization are diverse. We proposed a stroboscope-based method for analyzing driven chaotic systems in their phase space. According to two statistic quantities generated from time series, we could realize the system state and the driving behavior simultaneously. We demonstrated our method in a driven bi-stable system, which showed complex period windows under a proper driving force. With increasing periodic driving force, a route from interior periodic oscillation to phase synchronization through the chaos state could be found. Periodic windows could also be identified and the circumstances under which they occurred distinguished. Statistical results were supported by conditional Lyapunov exponent analysis to show the power in analyzing the unknown time series.

Dr. Li-Ling Yang (Institute of Physics, Academia Sinica; E-mail: lly.taiwan@gmail.com)
Talk Title: Revealing Min protein interactions in E. coli by dual-colour FCCS measurement
Abstract: Min protein system assists in septum determination during cell division in Escherichia coli by forming the dynamic concentration gradient of MinC protein from the pole to mid-cell region. It is not only to assure that cell division occurs in the middle of cells, but also inhibit segregation in the pole region. Via the interplay between membrane-bound proteins, MinD and MinE, and cell membrane, the dynamic gradient is achieved in the form of concentration oscillation from one pole to the other. We are interested in the molecular mechanism of MinD/E interactions, and applied dual-colour fluorescence correlation spectroscopy (dcFCCS) to studying dynamics of MinD/E. Fluorescence correlation spectroscopy (FCS) is a powerful experimental technique by statistical analysis of equilibrium fluctuations of fluorescence emission based on confocal microscope. It could provide high spatial and temporal analysis on low-concentration biomolecules, even to single-molecule level. Parameters, such as mobility, concentration and rate constants, are obtainable with the FCS/dcFCCS measurement. It can be applied not only to a simple homogenous solution but also to cells, membranes and whole organisms. Furthermore, by introducing the second imaging colour and cross-correlation (dcFCCS) analysis, interactions between molecules in terms of binding ratio can also be determined.

From our measurements, the trend of MinD-MinE complex ratio is a cycle of oscillation was firstly built up, and further information was provided. On the one hand, there existed MinE protein bound to membrane without its MinD binding partner. This suggested that MinE might have also binding affinity to the cell membrane even in the absence of MinD. On the other hand, the MinD-MinE complex ratio followed the concentration wave of MinE, and was getting up and down in a oscillation cycle. Surprisingly, the MinD-MinE complex ratio was not totally depleted in the dip region, and remained some dregs of complex. It infers that the oscillation process mainly proceeds with the stochastic diffusion-reaction process rather than forming complex filaments. These direct observations on association-disassociation process of MinD/E and membrane in vivo would advance our understanding to the interaction mechanism.

Dr. Chun-Ling Chang (Institute of Physics, Academia Sinica; E-mail: cichang@phys.sinica.edu.tw)
Talk Title: Temporal behavior of DNA thermal stability in the presence of platinum compounds. Role of monofunctional and bifunctional adducts
Abstract: Penetrating into cell nuclei, antitumor drug cisplatin sequentially forms various intermediate and final adducts destroying local DNA structure. The demonstrated disappearance of the fine structure of melting curve of long DNAs along with a strong decrease in melting enthalpy conforms to the structural impact. However, the negative thermal effect (δTm) caused by cisplatin is relatively small if neutral medium is used in melting experiments. Cisplatin’s inactive analogs transplatin and diethylenetriaminechloroplatinum (Pt[(dien)Cl]Cl) also distort DNA structure but their thermal effect is even positive. We have found that the use of alkaline medium inmelting experiments strengthens the negative thermal effect for cisplatin. For transplatin and Pt[(dien)Cl]Cl, the thermal effect becomes negative that makes it qualitatively consistent with structural
distortions. Those changes are explained by elimination of nonspecific electrostatic stabilization of DNA under platination. Additionally, alkaline medium fixes intermediate states of DNA platination and makes them stable against heating. These results allowed us to monitor $\delta T_m$ under binding of platinum compounds to DNA and their further transformation. The kinetic and thermal characteristics of monofunctional and bifunctional adducts were evaluated. It has been demonstrated that monofunctional adducts of cisplatin, transplatin and Pt[(dien)Cl]Cl produce approximately the same thermal destabilization. Cisplatin intrastand crosslinks cause a two-fold stronger thermal destabilization than its monofunctional adducts. The value of $\delta T_m$ for cisplatin's final adducts is ten times larger than for transplatin. This difference mainly comes from the much stronger thermal destabilizing power of cisplatin's intrastand crosslinks, which are responsible for antitumor activity of this compound.

Ms. Pei-Yin Chi (Nano Science and Technology, Taiwan International Graduate Program, Academia Sinica; Department of Engineering and System Science, National Tsing Hua University; & Institute of Physics, Academia Sinica; E-mail: cpy@phys.sinica.edu.tw)

Talk Title: Characterizing nucleus deformation of cancer cells through microfluidic slit orifice

Abstract: For cancer metastasis to occur, a cancer cell must perform transmigration, i.e. it has to invade the interstitial tissues either through bodily fluid circulation, or by direct movement, possibly overcoming one or more obstacles, such as the basement membrane. The process of migration costs energy and requires that the migrating cell's cytoplasm and organelles deform to pass through the openings smaller than the cell diameter. The size of these openings depends on the sterical arrangement of the ECM, density of the basement membrane, and other properties of the tissue through which the cancer cell migrates. It turns out that the most important limiting factor in this process of transmigration is the deformation of the nucleus. The nucleus is 5-10 times stiffer than the cytoplasm and the nuclear deformation is the rate limiting factor for the cell transmigration in the dense connective tissue.

Here we present a microfluidic device to study the cell migration through openings that require the cell nucleus to deform. The device has parallel cell incubation channels connected by transversal slits with dimensions ranging from 250 nm−2 µm vertically and 5–50 µm horizontally. The slits also serve to confine the studied phenomenon to the focal plane of an optical microscope, facilitating detailed observation of the temporal sequence of the nucleus deformation events. A special feature of our chip design is that we can synchronize the observation by mechanically gating the slits closed and open at a given time. The features of our chip serve to precisely control of the physical and chemical parameters of the experimental system used to study the nuclear deformation of a migrating cell.

We co-cultured lung cancer cells (CL1-0) and lung fibroblasts (MRC-5) in the parallel cell incubation channels of the chip. The fibroblasts in one channel serve to attract the cancer cells in the other to induce transmigration. We have observed cancer cell transmigration through a slit with 1 µm height and 100 µm width, requiring deformation of the nucleus of the migrating cell. At the beginning, the cytoplasm protrudes and explores into the slit. The cell protrusions then elongate all the way across the slit to the channel incubated with fibroblasts, and most of the cell cytoplasm quickly passes to the other side, leaving the nucleus with the remaining portion of the cytoplasm at the slit entrance. After this, there is a delay during which the cell tries to "fit" the nucleus into the slit opening. Finally, the nucleus deforms and quickly passes across the 50 µm distance to the side with fibroblasts. The whole process takes about 3-5 hours. The migration sequence of the cytoplasm and organelles of the cell can be clearly observed. For the slit with vertical dimension less than 0.5 µm, penetration of the cytoplasmic protrusions across the slit can still be observed, but not the nucleus. If the slit length was too long, the cancer cell nucleus will not deform and transmigrate to the other channel. In this case, the cytoplasm extends to 150 µm long into the slit of 1 µm height. During the nucleus deformation, the observed physical factors, such as speed, elasticity, and compartmentalization can be characterized. Our chip provides a versatile platform to study the nucleus deformation, organelle migration sequence, and organelle deformation during cell transmigration by direct visualization. Further research opportunities provided by this platform may include the study of mechanical forces, gene expression, protein regulation, and nucleus matrix during nuclear deformation.

Mr. Guan-Rong Huang (Department of Physics, National Taiwan University; E-mail: r99222064@ntu.edu.tw)

Talk Title: The Biological Chemical Master Equation

Abstract: Stochastic dynamics in biophysics is active in the recent years. The stochastic differential equation (SDE), chemical master equation (CME), is widely used to explain the biological reaction mechanism. Here we will introduce the Van Kampen CME, the combination of Van Kampen equation and Fokker-Planck equation, and give their analytical solution and a numerical method to simulate it. The simulated solution is consistent with the analytical solution when the time is in large scale.
Mr. Xuhui Xiao (Department of Physics, National Taiwan University; E-mail: maat361@yahoo.com.tw)
Talk Title: *A simplified lattice model for polypeptide fibril transitions*
Abstract: Polypeptide fibril transitions are studied using a simplified lattice model, modified from the three-state Potts model, where uniform residues as spins, placed on a planar rectangular lattice, can interact with neighbors to form coil, helix, sheet, or fibril structure. Using the transfer matrix approach and numerical calculation, we analyzed the partition function and construct the phase diagram. The model manifests phase transitions among coil, secondary structures, and fibril through parameterizing bond coupling strengths and structural entropies of helix, sheet, and fibril states. The phase diagram shows the transition sequences are governed by the structural entropies, while the transition temperature is determined by the bond coupling strengths. The average fractional content and heat capacity of each structure are also analyzed.

Ms. Yu-Hsin Hsieh (Department of Physics, National Taiwan University; E-mail: d99222007@ntu.edu.tw)
Talk Title: *Heat capacity components carried by partition function zeros in interacting self-avoiding walks*
Abstract: The aim of this report attempts to demonstrate a new idea about how to associate partition function zeros with thermodynamic functions. The model which we adopt is the interacting self-avoiding walk (ISAW) on the simple cubic lattice. We calculate the exact partition function up to 27 monomers and determine the heat capacity components, which can be used to identify the order of the freezing transition and the collapse transition of the ISAW model. By considering the end-to-end distance of the ISAW, we could obtain more accurate critical points by finite-size extrapolation. It is hoped that the heat capacity decomposition method can serve as a new general method for the study of phase transition and critical phenomena.