KMI Theory Seminar

Friday, February 28, 2014
3:00 pm, KMI Science Symposia (ES635)

"Statistical Mechanics without Ensembles --- Thermal Pure Quantum Formulation"

Akira Shimizu
The University of Tokyo, Komaba

Abstract:

Statistical mechanics is conventionally given in the ensemble formulation, in which an equilibrium state is given by a mixed quantum state, which is represented by a density operator (Gibbs state). By contrast, we formulate statistical mechanics based on a pure quantum state, which we call a thermal pure quantum (TPQ) state [1-3]. A single TPQ state gives equilibrium values of all quantities of statistical-mechanical interest, i.e., it gives not only mechanical variables, such as magnetization and correlation functions, but also genuine thermodynamic variables and thermodynamic functions, such as entropy and free energy. In this TPQ formulation, thermal fluctuations are completely included in quantum-mechanical fluctuations. As a consequence, TPQ states have much larger quantum entanglement than the equilibrium density operators of the ensemble formulation [4]. We also show that the TPQ formulation is very useful in practical computations, by applying the formulation to quantum spin systems [1, 2] and to a strongly-interacting fermion system [3].

[1] S. Sugiura and A. Shimizu, Phys. Rev. Lett. 108, 240401 (2012).
[2] S. Sugiura and A. Shimizu, Phys. Rev. Lett. 111, 010401 (2013).
[3] M. Hyuga, S. Sugiura, K. Sakai and A. Shimizu, in preparation.
[4] S. Sugiura and A. Shimizu, arXiv:1312.5145.