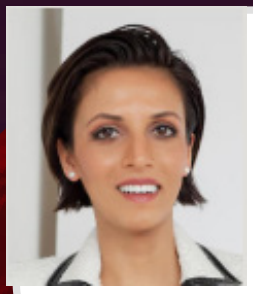
# Oral Session A2 (Tuesday, February 13)

**Chair: Stefan Blügel,**
**Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich GmbH**

## Keynote Talk



**14: 00 - 14 : 40**

### Prineha Narang

Physical Sciences, the University of California, Los Angeles (UCLA)

### TBD

## Contributed Oral

**14 : 40 - 15: 00**

### Hyperuniform electron distribution in quasicrystals

**Shiro Sakai**
RIKEN Center for Emergent Matter Science, Japan

Electrons in a quasiperiodic potential or lattice are distributed in an aperiodic but regular manner. Although electron wavefunctions in such a system often show multifractality, other physical quantities do not necessarily have multifractal distribution. For instance, the charge distribution on a Penrose lattice is not multifractal but hyperuniform [1].
Hyperuniformity [2] is a framework to quantify the regularity of a point distribution in a *d*- dimensional space. Counting the number of the points inside a window of radius R, we define its variance$\sigma^2$ ($R$) as the window moves over the space. The distribution with$\sigma^2$ ($R$) < O($R^d$) is called hyperuniform, as it is more uniform than a random distribution. Several different hyperuniformity classes have been identified.

Using a generalization of the hyperuniformity framework to scalar fields [2], we studied a one-dimensional Aubry-Andre-Harper model in terms of hyperuniformity [3]. The charge distribution of this model was found to be either class-I or class-II hyperuniform depending on the model parameters. By calculating the total energy, we found a phase transition between the regions of different hyperuniformity classes. This is a transition between two different non-uniform charge distributions in the absence of translational symmetry

**Referemces**

[1] S. Sakai, R. Arita, and T. Ohtsuki, Phys. Rev. B **105** (2022), 054202.
[2] S. Torquato, Phys. Rep. **745** (2018), 1.
[3] S. Sakai, R. Arita, and T. Ohtsuki, Phys. Rev. Research **4** (2022), 033241.

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## Contributed Oral

**15: 00 - 15: 20**

### Four-index coulomb interaction beyond Hund's coupling

**Steffen Backes**
RIKEN iTHEMS

To study the properties of strongly correlated electron materials one usually employs an effective low-energy lattice model, such as the Hubbard model, to obtain a simplified description of the material under consideration. Such a model is fully defined by the kinetic, or electron-hopping term, and the interaction term, originating from the electron-electron Coulomb interaction. This interaction term is a two-particle operator and in general involves the interaction of 4 different electron channels. For highly symmetric orbital basis functions this term is sparse and involves terms like the density-density interaction, or pair-hopping and spin-flip terms induced by the Hund's coupling. Even though in real materials all 4-index terms can in principle provide a finite contribution, they are usually assumed to be small and thus neglected for most practical calculations.
In this talk we will discuss the symmetry constraints imposed by the symmetry group of the corresponding atom on the form of the Coulomb interaction, and how the resulting non-zero elements can be obtained for specific systems. Using the constrained random-phase approximation we will present ab-initio 4-index elements of the Coulomb interaction for real materials and discuss cases where they show a non-negligible effect on the electronic structure. Using exact diagonalization of finite systems and the dynamical mean-field theory for lattice models and real materials, we will present the impact of these terms on electronic properties such as the spectral function.

## Contributed Oral

**15: 20 - 15: 40**

### Exact quantum spin Hamiltonian for magnetic interactions

**H. Katsumoto**[1], F. Lux[2], Y. Mokrousov[1,3], and S. Blügel[1]

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2 Department of Physics, Yeshiva University, USA
3 Institute of Physics, Johannes Gutenberg-University Mainz, Germany

The intricate nature of magnetism arises from the interplay of Heisenberg interactions and higher-order exchange interactions [1, 2]. The awareness is rising that the higher-order exchange interactions depend not only on the number of magnetic sites $N$ but also on the local spin magnitude $S$. Nevertheless, a definitive method for uniquely deriving a spin Hamiltonian that comprehensively captures these interactions for a given system remains elusive.

his presentation is dedicated to delving into the algebraic aspects of the spin-permutation operator offering a methodology for deriving an exact quantum spin Hamiltonian tailored for an $N$- site system of spin $S$. We showcase the construction of the exact quantum spin Hamiltonian of $S = 1/2$ and 1 and extending to higher-order interactions up to 4-site systems. Furthermore, we delve into higher-order terms related to scalar spin chirality using this algebraic approach. he magnetism in solid materials is described by the classicalization of the quantum spin Hamiltonian.

hese findings not only contribute to our understanding of magnetism in solids but also bear relevance to nuclei and cold atom systems.

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**References**

[1] M. Hoffmann et al., Phy. Rev. B 101, 024418 (2020).
[2] S. Grytsiuk et al., Nat. Commun. 11, 511 (2020).