Summary of recent work

May 11, 2020

Sparse modeling approach to many-body problems

In this subsection, I summarize a collection of my recent works on sparse modeling approach to many-body problems. Sparse modeling refers to methodologies for finding a small number of relevant parameters that well explain a given dataset, being widely used for signal processing such as image denoising. These methodologies have two important ingredients. The first one is a sparse basis for signals in which the projected data has only a few non zero elements. The second one is regularized fitting techniques that enables to separate the true signal from noise in that basis.

In [8], we found a new compact/sparse basis for representing the frequency dependence of Matsubara Green's function, which was named as "Intermediate representation" (IR). In [9], we developed a stable method for analytic continuation of imaginary-time data to a spectral function based on this compact basis and sparse sampling techniques. In [5], we used the newly proposed analytic continuation method to denoise the self energy obtained by an exact diagonalization solver in dynamical mean-field calculations. These papers are reviewed in Sections 5, 6, 7 of the invited review article [1].

In 2017, we found that the compactness of the IR basis was potentially useful for many-body calculations based on Matsubara Green's function. In [4], we proposed "sparse sampling techniques" that enables to accelerate many-body diagrammatic calculations at the single-particle level such as GW calculations. In [2], this method was soon applied to *ab initio* Migdal-Eliashberg calculations to consider retardation effect in phonon-mediated superconductors. Paper [6] describes our open-source implementation of the IR basis in Python/C++, which was used in our studies.

In [7] and [3], we extended the IR basis and the sparse sampling techniques to two-particle Green's functions. In [3], we also proposed a tensor network representation of two-particle Green's functions, which are essentially a multi-dimensional tensor data in terms of spins, orbitals, Matsubara frequencies. The tensor network representation greatly reduces the storage size of two-particle data by a several orders of magnitudes. In [3], we demonstrated efficiency of the scheme for calculations of static and dynamic susceptibilities in single- and two-band Hubbard models in the framework of dynamical mean-field theory.

We are still actively working on these issues and are trying to use these techniques to perform self-consistent diagrammatic calculations at the two-particle level in collaboration especially with Karsten Held's group at TU-Wien in Austria. This will open a route to the application of modern many-body theories to realistic strongly correlated electron systems such as parquet approximation, dynamical vertex approximation, and dual-fermion approach.

1. **(Invited review paper)** J. Otsuki, M. Ohzeki, H. Shinaoka, and K. Yoshimi, JPSJ **89**, 012001 (2020)
2. T. Wang, T. Nomoto, Y. Nomura, H. Shinaoka, J. Otsuki, T. Koretsune, R. Arita, arXiv:2004.08591
3. H. Shinaoka, D. Geffroy, M. Wallerberger, J. Otsuki, K. Yoshimi, E. Gull, Jan Kuneš, SciPost Phys. **8**, 012 (2020)
4. J. Li, M. Wallerberger, N. Chikano, C.-N. Yeh, E. Gull, and H. Shinaoka, PRB **101**, 035144 (2020)
5. Y. Nagai and H. Shinaoka, JPSJ **88**, 064004 (2019)
6. N. Chikano, J. Otsuki, and H. Shinaoka, PRB **98**, 035104 (2018)
7. H. Shinaoka, J. Otsuki, K. Haule, M. Wallerberger, E. Gull, K. Yoshimi, and M. Ohzeki, PRB **97**, 205111 (2018)
8. H. Shinaoka, J. Otsuki, M. Ohzeki, and K. Yoshimi, PRB **96**, 035147 (2017)
9. J. Otsuki, M. Ohzeki, H. Shinaoka, and K. Yoshimi, PRE **95**, 061302(R) (2017)

Contributions to ALPS project

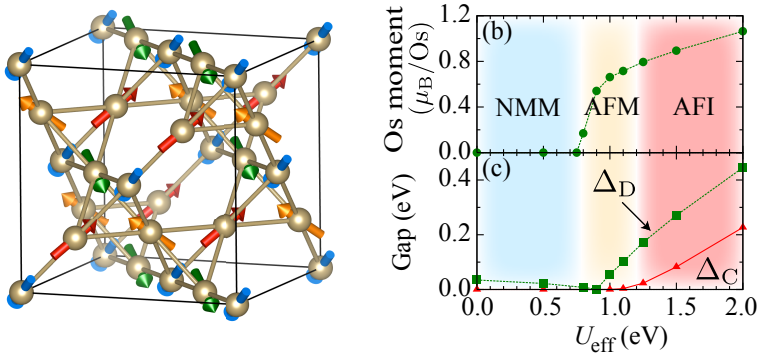
I have been contributing to the development of many open-source softwares in the ALPS (Algorithms and Libraries for Physics Simulations) project. I contributed some codes to the core library of ALPS [1] and developed new efficient continuous-time Monte Carlo codes based on the hybridization expansion algorithm [2] and the interaction expansion algorithm [3] as the main developer. The ALPS library has been widely used for physical simulations all over the world for many years. The ALPS/CT-HYB [2] is efficient and optimized for solving a multi-orbital impurity problem with general onsite interactions. This code is suitable for computing real materials or multi-orbital Hubbard models by the dynamical mean-field theory.

1. A Gaenko, A E Antipov, G Carcassi, T Chen, X Chen, Q Dong, L Gamper, J Gukelberger, R Igarashi, S Iskakov, M Könz, J P F LeBlanc, R Levy, P N Ma, J E Paki, H Shinaoka, S Todo, M Troyer, and E Gull, Comput. Phys. Commun. **213**, 235 (2017)
2. H. Shinaoka, E. Gull, P. Werner, Compt. Phys. Commun. **215**, 128 (2017)
3. H. Shinaoka, Y. Nomura, E. Gull, to appear in Compt. Phys. Commun (arXiv:1807.05238)

First-principles study of metal-insulator transition and noncollinear magnetism in $Cd_2Os_2O_7$

It is experimentally known that the pyrochlore oxide Cd2Os2O7 exhibits a metal-insulator transition accompanied by antiferromagnetic ordering around 225 K. However, the nature of the low temperature phase, including its magnetic structure, has not been well understood in spite of more than 30 years of research.

I have shown by relativistic first-principles calculations that the non-collinear magnetic state (right figure), called the all-in/all-out type, is stable as the ground state. Furthermore, the easy axis anisotropy along the local [111] axis stabilizes the magnetic structure. In the vicinity of the antiferromagnetic metal-insulating phase boundary, the band structure is semimetallic and the pseudo-gap structure appears in the density of states. These results explain the experimentally observed low temperature properties of the material.

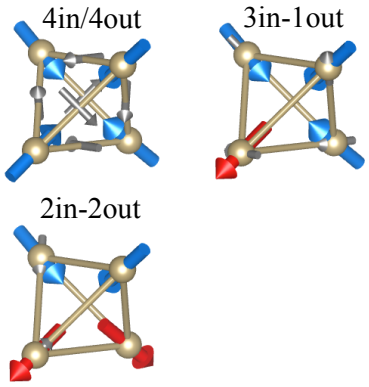


1. **(Topical review)** H. Shinaoka, Y. Motome, T. Miyake, S. Ishibashi and P. Werner, Journal of Physics: Condensed Matter, **31** (2019)
2. H. Shinaoka, T. Miyake, and S. Ishibashi, PRL **108**, 247204 (2012)

First-principles study of spin-orbital frustration in Mo pyrochlore oxides

The pyrochlore oxide A2Mo2O7 is a typical 4d transition metal oxide that exhibits a metal-insulator transition. In particular, insulating materials (A=Y, Tb, etc.) are known for their peculiar magnetic properties, such as the spin-glass transition instead of long-range magnetic ordering at low temperatures. Traditionally, these materials have been regarded as typical geometrically frustrated magnets with isotropic nearest-neighbor antiferromagnetic interactions between spins arranged on a pyrochlore lattice. However, recent neutron scattering experiments have revealed that the spin correlations at low temperatures do not agree with the conventional theory. Contrary to previous theories based on the antiferromagnetic spin model, the development of ferromagnetic spin correlations has been observed, and a complete reconsideration of the microscopic origin of magnetic competition is required.

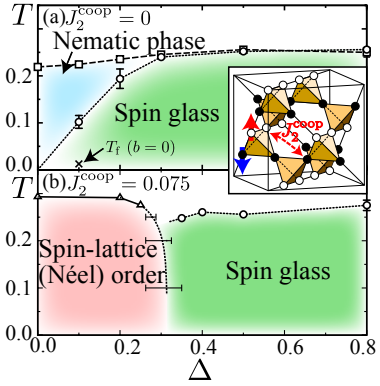
As a result of relativistic first-principles calculations, I found that different insulating states with antiferromagnetic and ferromagnetic magnetic structures compete as ground states, as shown in the right figure. An effective spin model based on first-principles calculations is investigated, and it is found that the singular degeneracy is the result of anisotropic spin interactions in the spin space. It is shown by classical Monte Carlo calculations that the system is located near the phase boundary between ferromagnetic and antiferromagnetic insulating phases and that ferromagnetic spin correlations can develop due to small changes in the interaction parameters. To investigate the microscopic origin of magnetic anisotropy, a first-principles multi-orbital Hubbard model based on the most localized Wannier function is analyzed. The results show that magnetic competition are related to competition between different orbital orders. These results overturn the conventional spin-glass picture based on an isotropic antiferromagnetic spin model and fully explain the latest experimental results.



1. **(Topical review)** H. Shinaoka, Y. Motome, T. Miyake, S. Ishibashi and P. Werner, Journal of Physics: Condensed Matter, **31** (2019)
2. H. Shinaoka, Y. Motome, T. Miyake, and S. Ishibashi, PRB **88**, 174422 (2013)

Spin-glass Transition in disordered geometrically frustrated magnets coupled with local lattice distortion

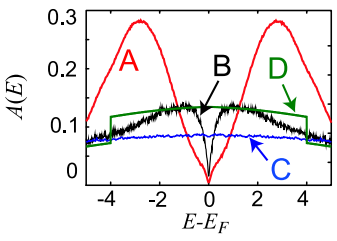
The spin glass phase, in which the spin is randomly frozen, is one of the cold phases widely found in geometrically frustrated magnetic materials. In some pyrochlore antiferromagnets [Y2Mo2O7, etc.], a spin glass transition is observed at relatively high temperatures even in less disturbed samples, and the transition temperature is almost independent of the intensity of the disturbance. These strange behaviors have been observed in many frustrated magnetic materials.



I have shown that the peculiar spin glass behavior can be understood as the effect of the coupling between spin and local lattice distortion. Specifically, the phase diagram of the antiferromagnetic Heisenberg spin model on the pyrochlore lattice was studied by classical Monte Carlo calculations, and it was found that the spin glass transition temperature was greatly increased by the spin-lattice coupling. In the strongly disordered region, the spin glass transition temperature is determined by the strength of the spin-lattice coupling, being almost independent of the strength of disorder. These explain the unusual spin glass behavior commonly found in geometric frustrated systems.

1. H. Shinaoka, Y. Tomita, and Y. Motome, PRL **107**, 047204 (2011)
2. H. Shinaoka, Y. Tomita, and Y. Motome, PRB **90**, 165119 (2014)

Unconventional single-particle excitation spectrum induced by coexisting randomness and strong electron correlation



The insulator due to electron correlation has a gap in the density of states excited by one particle, while the disorder-induced Anderson insulator has a finite value of the density of states above the Fermi level. The excitation structure realized when these two effects coexist is a fundamental and unobvious unsolved problem in condensed matter physics.

I introduce the disturbed on-site potential into the three-dimensional Hubbard model and analyze the ground state within the real space Hartley Fock approximation. As a result, in the insulating phase where turbulence and electron correlation coexist, we found a "soft gap" structure in which the 1-particle excited state density disappears only at the Fermi level. This cannot be explained by the conventional theory that the soft gap is formed

from the effect of the long-range Coulomb interaction. I have clarified from the phenomenological theory that the soft gap structure appears when low-energy many-body excited states exist due to the competition between electron correlation and turbulence. The calculation based on the mean field approximation and the exact diagonalization method was also carried out in the case of 1 and 2 dimensions, and the result indicating the soft gap structure was obtained.

1. H. Shinaoka and M. Imada, PRL **102**, 016404 (2009)
2. H. Shinaoka and M. Imada, JPSJ **78**, 094708 (2009)