Development of many-body variational Monte Carlo method and its application to correlated topological phases

(Oral)

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Strong electron correlations in solids are the source of various exotic quantum phases, such as high-T_c superconductivity and quantum spin liquids. Clarifying how strong electron correlations induce these exotic quantum phases is one of the central issues of modern condensed matter physics. To accurately analyze the effects of electron correlations, we have developed a many-variable variational Monte Carlo (mVMC) method [1]. In this method, we use trial wave functions with over 10^4 variational parameters and optimize them. This mVMC method enables a highly accurate analysis of effective models of strongly correlated electron systems. We have applied the mVMC method to a wide range of strongly correlated electron systems, such as *ab initio* low-energy effective models of iron-based superconductors [2], cuprates [3], and organic compounds [4-6].

In this talk, we will demonstrate the applications of mVMC method to correlated topological insulators. One example is a magnetic Chern insulator in the Kondo lattice model on a triangular lattice [7]. Using the mVMC method, we have shown that the triple-Q magnetic order becomes the ground state in an intermediate Kondo coupling region. By explicitly calculating the many-body Chern number using the twist operator method, we have shown that the many-body Chern number becomes one.

Another example is an unprecedented topological insulator in organic compound κ-(BEDT-TTF)$_2X$, which is one of the *textbook materials* of the Mott insulator, almost without spin-orbit coupling [8]. We have discovered that the celebrated Su-Schrieffer-Heeger model emerges, and the resultant spin-polarized edge states appear in the antiferromagnetic Mott insulating state. Using the mVMC method, we have demonstrated that this topological state is robust against electron correlation and quantum effects beyond the mean-field level by explicitly calculating the many-body Zak phase.

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