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A liquid-gas transition in a 3D Kitaev model

JOJI NASU, Tokyo Institute of Technology

Quantum spin liquid (QSL) is an exotic quantum state of matter in insulating magnets, where long-range ordering is suppressed down to the lowest temperature. Several experimental candidates of QSL have been recently nominated thus far. In their characterization, the absence of thermodynamic anomalies, namely, adiabatic connection from the high-temperature paramagnet (spin gas), is regarded as a hallmark of QSL. Although adiabatic connection between liquid and gas is allowed by bypassing the critical end point in conventional fluids, it is highly nontrivial whether a thermodynamic transition between QSL and paramagnet exists or not in quantum spin systems. The issue is crucial not only for theoretical understanding of QSLs but also for the interpretation of existing and forthcoming experiments. To clarify this problem, we investigate a three-dimensional extension of the Kitaev model [1,2,3]. This model is relevant to the recently found Ir oxides Li_2IrO_3 . The Kitaev model is one of the solvable quantum spin models, where the ground state is given by gapped and gapless QSLs, depending on the anisotropy of the interactions. This model can be rewritten as a free Majorana fermion system coupled with \mathbb{Z}_2 variables. Using this representation, we perform the Monte Carlo simulation and analyze the thermodynamic properties. We find that the model exhibits a finite-temperature phase transition between the QSLs and paramagnet in the whole parameter range. This result indicates that both gapless and gapped QSL phases at low temperatures are always distinguished from the high-temperature paramagnet by a phase transition. We also find that the difference between QSL and paramagnet comes from the topological nature of the excitations. This work has been done in collaboration with Y. Motome and M. Udagawa in Univ. of Tokyo. [1] J. Nasu, M. Udagawa, and Y. Motome, Phys. Rev. Lett. **113** 197205 (2014). [2] J. Nasu *et al.*, Phys. Rev. B **89** 115125 (2014). [3] J. Nasu, M. Udagawa, and Y. Motome, preprint (arXiv:1409.4865).