Bayesian investigation of quantum criticality in spin dimer systems

Stephan Allenspach,1,2 Alexander Madsen,1,3 Pascal Puphal,4 Steffen Krämer,5 Mladen Horvatić,5 Raivo Stern,6 Maciej Bartkowiak,7 Oleksandr Prokhnenko,7 Nicolas Laflorencie,8 Frédéric Mila,9 Bruce Normand,1,9,10 and Christian Rüegg,1,2,9,11

1 Quantum Criticality and Dynamics Group, Paul Scherrer Institute, CH-5232 Villigen-PSI, Switzerland
2 Department of Quantum Matter Physics, University of Geneva, CH-1211 Geneva, Switzerland
3 Institute of Computational Science, Università della Svizzera italiana, CH-6900 Lugano, Switzerland
4 Max Planck Institute for Solid-State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany
5 Laboratoire National des Champs Magnétiques Intenses, LNCMI-CNRS (UPR3228), EMFL, Université Grenoble Alpes, UPS and INSA
6 National Institute of Chemical Physics and Biophysics, 12618 Tallinn, Estonia
7 Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Lise Meitner Campus, Hahn-Meitner-Platz 1, 14109 Berlin, Germany
8 Laboratoire de Physique Théorique, CNRS and Université de Toulouse, 31062 Toulouse, France
9 Institute of Physics, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland
10 Lehrstuhl für Theoretische Physik I, Technische Universität Dortmund, Otto-Hahn-Straße 4, 44221 Dortmund, Germany
11 Institute for Quantum Electronics, ETH Zürich, CH-8093 Hönggerberg, Switzerland

Phase transitions and their accompanying concepts of criticality and universality are a foundation stone of statistical physics. In gapped spin dimer systems a quantum phase transition can be induced by applying a magnetic field. At this transition $U(1)$ symmetry is broken and the resulting field-induced phase corresponds to a Bose-Einstein condensate (BEC) of magnetic quasi-particles. The phase boundary takes the functional form $T_c(H) = \alpha \left[\mu_0 H - \mu_0 H_{c1}\right]^\phi$ in the critical regime for these systems and the exponent $\phi = 2/d$ can be used to determine the dimensionality, $d$, of the BEC. However, determining $\phi$ from data is challenging due the high correlation between the parameters ($\phi, H_{c1}, \alpha$) and because the size of the critical regime is non-universal and unknown.

Bayesian Inference (BI) is a statistical method used in various areas of physics [1]. The result of BI is not a point estimate but a probability distribution, called the posterior distribution, of the model parameters given the data. BI provides a systematic framework to estimate the value and uncertainty of any single parameter independently from all the other parameters by integrating them out of the posterior distribution. In addition, correlations between parameters are directly visible in the joint posterior distribution of these parameters. Thus using BI in an analysis of the phase boundary, the first problem of independently determining $\phi$ is solved.

We use BI to determine $\phi$ from Nuclear Magnetic Resonance spectra measured for the quasi-2D spin dimer compound $\text{Ba}_{0.9}\text{Sr}_{0.1}\text{CuSi}_2\text{O}_6$ [2]. By varying the range of the data included in the analysis, we tackle the second problem and find a value of $\phi = 2/3$ (3D). Additionally, we employ BI for the analysis of neutron diffraction data measured for the parent compound $\text{BaSrCuSi}_2\text{O}_6$ at magnetic fields up to 25.9 T.