Bayesian investigation of quantum criticality in spin dimer systems

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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 $T_c(H) = \alpha[\mu_0 H - \mu_0 H_{c1}]^{\phi}$ 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 ϕ from data is challenging due the high correlation between the parameters (ϕ, H_{c1}, α) 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 ϕ is solved.

We use BI to determine ϕ from Nuclear Magnetic Resonance spectra measured for the quasi-2D spin dimer compound $Ba_{0.9}Sr_{0.1}CuSi_2O_6$ [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 $BaSrCuSi_2O_6$ at magnetic fields up to 25.9 T.

[1] U. von Toussaint, Bayesian inference in physics, Rev. Mod. Phys. **83**, 943 (2011).

[2] S. Allenspach *et al.*, Revealing three-dimensional quantum criticality by Sr substitution in Han purple, Phys. Rev. Res. **3**, 023177 (2021).