Probing Quantum Discord in a Heisenberg Dimer Compound

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Abstract. Temperature dependent quantum correlations (quantum discord, total correlations and spin-spin pair correlation) between the microscopic constituents of a magnetic system comprising spin ½ particles have been estimated through experimentally measured macroscopic thermodynamic properties (magnetic susceptibility and specific heat) . Moreover, violation of Bell's inequality test has also been performed for the same compound using the experimental data.

Keywords: Spin Dimer. Quantum Discord

1 Introduction

Detection of quantum correlations in solid state bulk bodies through thermodynamic properties has fascinated the research in quantum information processing due to its significance in verifying several quantum computational protocols in various physical systems in the macroscopic scale [1]. Especially, entanglement has been recognized as very useful in several quantum computational aspects [2]. Despite being such a valuable entity, entanglement is unable to capture all non-classical correlations because even in the non-entangled (or separable) regime, the system can remain quantum mechanically correlated. The above mentioned issue was addressed by invoking a new quantity called Quantum Discord (QD) which by definition captures the "non-classicality" that encompasses entanglement as a subset [3]. It is a well established fact that QD can affect macroscopic properties like magnetic susceptibility in considerably low temperature regime. This implies that one can get a signature of QD between the microscopic constituents of a real material in the thermodynamic limit by only carrying out bulk magnetic measurements [4]. The present compound has been studied from the perspective of quantum information processing and the content of quantum correlations has been quantified from experimental data.

In the present paper, quantum correlations have been quantified for NH_4CuPO_4, H_2O. Crystal structure and magnetic properties have revealed the fact that the magnetic interactions in NH4CuPO4, H2O can indeed be described by isolated spin 1/2 Heisenberg dimer model [5]. Herein, QD and other correlations (mutual information and spin-spin pair correlation) have been quantified from experimental susceptibility and specific heat data and their variations are captured as a function of temperature.

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2 Experimental Details

Using $CuCl_2$, H2O and $(NH_4)_2HPO_4$ of the purest grade (obtained from Sigma Aldrich) as starting reagents, chemical synthesis and crystallization were performed and greenish blue prism shaped crystals were obtained. Subsequently, Temperature dependent static magnetic susceptibility measurements were carried out in a SQUID magnetometer (Magnetic Property Measurement System, Quantum Design) in a temperature range of 2-20K. Temperature dependent specific heat measurements were carried out in a range of 2-10K by standard relaxation technique in a cryogen free magnet.

3 Results and Discussions

Experimental susceptibility and specific heat data have been analyzed within the framework of spin ½ Heisenberg model. The theoretical fit yielded Landé g-factor g=2.11 and exchange coupling constant J=5K. Spin-spin correlation function (G) has functional dependence on magnetic susceptibility and specific heat data for a Heisenberg two qubit system. Now, G is empirically connected with mutual information (I) and classical correlation (Q) function which eventually provides an experimental measure of QD as QD is simply defined as QD=I-Q [3, 6]. Based on this theoretical treatment, we are now in a position to extract QD from experimental data. All the three correlations were extracted in the thermodynamic limit using the experimentally measured susceptibility and specific heat data. Quantified QD, I and Q are shown in FIG. 1. The graph clearly exhibits that QD along with the other three correlations attain their maximum value when temperature is minimum. As the temperature is increased, all the three correlations decrease gradually. As experimentally measured thermodynamic properties directly reveal material-specific macroscopic quantum correlations between the microscopic constituents of a given solid state material, quantified correlations signify the content of quantum correlations between the spins of the two-spin ½ cluster compound $NH_4CuPO_4.H_2O$. Indeed, this methodology is based on the criterion that NH4CuPO4.H2O is prototype of spin ½ Heisenberg dimer which has already been corroborated by the previous analysis on the experimental data. It is a necessary practice to check the validity of the experimentally quantified values by comparing with the relevant theoretical model. Hence, considering the dimer model, the density matrix and the quantum correlations are calculated by following the protocol described by Pal *et al.* [6]. Looking at the graph, one can conclude that the theoretical curves are well consistent with the quantified correlations from experimental data.

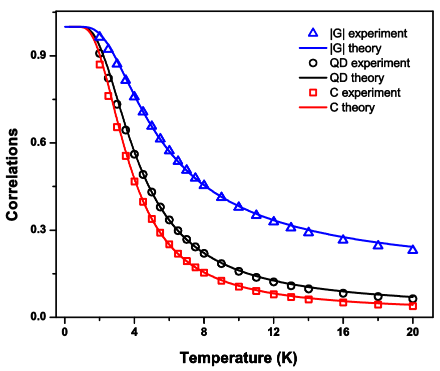

FIG. 1. Temperature dependent correlations |G| (triangles), QD (circles) and I (squares) quantified from susceptibility data. The solid lines represent the corresponding correlations calculated theoretically for Heisenberg dimer model.

Due to its fundamental significance in foundation of quantum mechanics, Bell's inequality test has been recognized as an efficient tool to examine the signature of entangled states in a two qubit system [8]. The mean value of the Bell operator |<B>| holds an empirical relationship with magnetic susceptibility and specific heat through G. violation of Bell's inequality is governed by the condition |<B>|>2 (the red line in FIG. 2) whereas |<B>|=2√2 indicates the maximal violation (the blue line in FIG. 2) [9]. Thus, the violation of Bell's inequality was tested by substituting the experimental data in the above equation. Extracted values of |<B>| are plotted in FIG. 2 as a function of temperature. Hence, for a real physical system, a Bell measurement combined with quantification of QD allows us to make the decisive statement that QD can survive persistently even in the region where Bell's inequality is not violated.

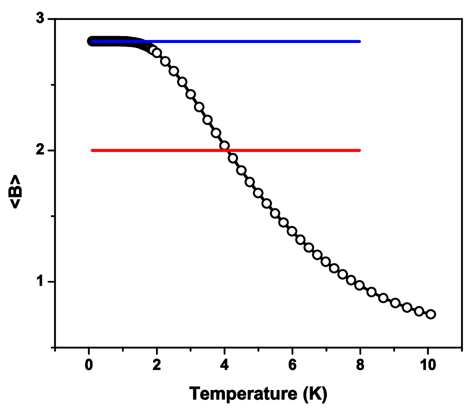

FIG. 2 Mean value of Bell operator (circles) as a function of temperature calculated from internal energy data. The blue and the red lines are the bounds as discussed in the text.

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