QUANTUM PHASE TRANSITIONS IN MAGNETIC SYSTEMS

by

Omid Nohadani

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Abstract

Phase transitions in quantum antiferromagnets offer exciting and novel insights into the critical behavior of matter at ultra-low temperatures.

In this thesis, we apply the stochastic series expansion quantum Monte Carlo method to study the critical properties of ensembles of antiferromagnetically coupled spins subject to quantum phase transitions. The zero-temperature phase diagram, describing various phase transitions induced by an applied magnetic field, is constructed. The corresponding quantum critical points are determined to highest accuracy, allowing a conclusive interpretation of recent experimental measurements. Moreover, the scaling properties of uniform magnetization and staggered transverse magnetizationin magnetic fields are calculated, allowing the determination of the universality class of the system. The associated critical exponents are derived from Ginzburg-Landau theory as well. We find excellent agreement between the quantum Monte Carlo simulations and the analytical results, as well as previous bond-operator calculations.

Furthermore, the critical scaling exponent, which governs the power-law dependence of the transition temperature on the applied magnetic field, is extracted from the numerical data. We show that this exponent is independent of material specific

inter-constituent interactions. Moreover, it converges to the value predicted for Bose-Einstein condensation of magnons. These results are of direct relevance to compounds such as $TlCuCl_3$ and $KCuCl_3$, and explain the broad range of exponents reported my exponents for field-induced ordering transitions.

Finally, we introduce geometric randomness into a model of coupled dimers. The calculations show that at finite randomness, field-induced quantum phase transitions into and out of ordered Bose-Einstein condensates pass through a Bose-Glass phase. The localization of the bosons and their finite compressibility manifests this unique regime. Once delocalized, the bosons condense, and long-range order sets in. We further detect that an intermediate magnetization plateau can occur for a parameter range, in which the spins of the doped bonds become fully polarized. This rich field-dependence is expected to be experimentally observable in weakly coupled dimer compounds with small doping and negligible spin-orbit coupling or directionality effects. The calculations in this thesis cover fundamental phases and transitions between them, as they can occur in antiferromagnetic quantum spin systems.

Chapter 7

Conclusions

In this thesis, quantum phase transitions in antiferromagnets were studied, using a combination of analytical and numerical techniques. Here, we summarize the results along with an outlook for possible investigation in the future.

The zero-temperature phase diagram of three-dimensional coupled dimer-spin systems was constructed using stochastic series expansion quantum Monte Carlo simulations. We developed massively parallel codes to simulate systems with up to 10,000 spins on more than 1,200 CPUs simultaneously, to warrant for the highest accuracy and reliable Monte Carlo results. In principle, stochastic series expansion quantum Monte Carlo calculations are finite-temperature simulations. In order to explore and understand the behavior of a large ensemble of spins in applied magnetic fields at ultra-low temperatures, we implemented the novel directed-loop algorithm. This effort unveiled the ultra-low temperature behavior of antiferromagnets through quantum Monte Carlo calculations. The resulting phase diagram

featured a low-field dimer spin liquid phase at weak inter-dimer couplings, a partially polarized regime with long-range transverse magnetic order for intermediate magnetic fields $h_c \leq h \leq h_s$, and a fully polarized phase at high magnetic fields. Both of these field-induced quantum phase transitions were shown to be continuous. The numerical values of these exponents agree perfectly with the presented Ginzburg-Landau calculations as well as previous bond-operator mean-field theory. Moreover, the quantum critical point is determined to highest accuracy, such that we could demonstrate cubic scaling for $m_u \propto h^3$ at the quantum critical point, as it was reported recently from magnetization study on the $TlCuCl_3$ compound under hydrostatic pressure. Furthermore, for the first time we present corrections to mean-field scaling, emerging at the zero-field pressure-induced quantum phase transition in three-dimensional compounds. In particular, we show that the experimental data from Ref. [81] can be well fitted to a mean-field scaling law taking into account logarithmic corrections.

With the knowledge of the universality class of these systems, the temperature dependence of the field-induced phase transition was investigated. We showed that the critical scaling exponents, describing the power-law of the transition temperature close to the critical field h_c (h_s), are independent of the inter-dimer coupling ratio. This demonstrates that, despite large quantitative differences in their magnon dispersion relations, the physical properties of the coupled-dimer systems, such as $KCuCl_3$ or $TlCuCl_3$, display the same universal scaling behavior. The exponents are consistent with a description of the ordering transitions as the Bose-Einstein condensation of magnon excitations. The extraction of the exponents was shown

to depend sensitively on the interval of data taken into account. We propose a novel technique to extract power-law exponents independent of the range of available data points. This method offers an explanation for the wide range of scaling exponents reported in current literature. Following our report, recent theoretical predictions as well as experimental measurements agree well with our calculations. [75, 74, 76] Several new compounds with different geometries and dimer arrangements were examined in high magnetic fields, confirming the presented calculations in this thesis.

Furthermore, we introduced randomness into a model of coupled dimers. The phase diagram found to be rich for weakly coupled dimers with random intra-dimer coupling strengths. Quantum Monte Carlo data shows that at finite randomness, a field-induced quantum phase transition into and out of an ordered Bose-Einstein condensate passes through a Bose-Glass phase. We clearly identify that the localization of the bosons and the finite compressibility manifests this unique regime. Once delocalized, the triplons condense and Néel-order sets in. We further detect that depending on coupling ratios, an intermediate plateau can occur, in which the spins of the doped bonds are fully polarized. This rich field-dependence is expected to be experimentally observable in weakly coupled dimer compounds with small doping and negligible spin-orbit coupling or directionality effects. We showed that Bose-Glass phases can occur in spin systems using the microscopic Heisenberg model.

For future investigations, we are eager to understand the competition of thermal and geometrical randomization close to quantum critical points. On the one hand,

temperature drives a quantum phase transition away from its pure quantum character. At the same time, the correlation between the space and imaginary time direction changes its exponent, as discussed in Chapter 3. On the other hand, geometric randomness at higher dimension may break the Harris criterion and thus become relevant for the critical exponents and subsequently for the universality class. The introduction of disorder could result in new phases created due to geometrical randomness, as reported in Chapter 6, the nature of which could be destroyed or changed upon the increase of temperature. In experimental studies, the real compounds are never 100% clean and always contain impurities, which could be modeled through geometrical disorder. At the same time, ultra-low temperature experiments require tremendous efforts and the laws of thermodynamics prevent zero-temperature measurements. Therefore, theoretical predictions of finite-temperature phase transitions in impurity doped or randomized quantum magnets would shine new light on these still not completely resolved questions.

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