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Spin transport in the two-dimensional quantum disordered anisotropic Heisenberg model

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ABSTRACT

We use the self consistent harmonic approximation together with the Linear Response Theory to study the effect of nonmagnetic disorder on spin transport in the quantum diluted two-dimensional anisotropic Heisenberg model with spin $S=1$ in a square lattice. The model has a *BKT* transition at zero dilution. We calculate the regular part of the spin conductivity $\sigma^{reg}(\omega)$ and the Drude weight $D_S(T)$ as a function of the non-magnetic concentration, x. Our calculations show that the spin conductivity drops abruptly to zero at $x_c^{SCHA} \approx 0.5$ indicating that the system changes from an ideal spin conductor state to an insulator. This value is far above the site percolation threshold $x_c^{site} \approx 0.41$. Although the *SCHA* fails in determining precisely the percolation threshold, both the spin conductivity and the Drude weight show a quite regular behavior inside $0 \le x \le x_c^{SCHA}$ indicating that the transition stays in the same universality class all along the interval.

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1. Introduction

The transport properties of materials are the corner stones for many applications. Once having these properties determined, it is possible to calculate the parameters for devices which can operate on the basis of these structures. Transport refers to the movement from one point to another induced by an external force. In a regular medium, propagation is ballistic: the average square of the distance covered after a time t scales like $\langle x^2(t)\rangle \propto v^2 t^2$ with v being the particle velocity. In a disordered medium containing impurities, the movement is no more ballistic. Quenched disorder is fixed for each realization of an experiment, but varies from experiment to experiment when samples are changed. Predictions about observables will involve an average over impurity configurations.

Recently, the spin transport phenomenon has attracted special attention due to its connection with spintronics [1]. The *XXZ* model, sometimes called the Quantum Anisotropic Heisenberg model (or quantum *XY* model), is a prototype for several magnetic materials and is of considerable interest in the context of statistical physics [2,3]. It can be obtained as the limit of several physical systems such as strongly correlated ultracold bosons in optical lattices or Josephson junction arrays [5–10]. It can also be used to describe the magnetic properties of some solid state materials [4]. The Mermin–Wagner theorem [11] predicts that there is no spontaneous broken symmetry in two dimensional systems with continuous symmetry. However, the pure (non-diluted) *XXZ* system undergoes a Berezinskii–Kosterlitz–Thouless, *BKT*, transition at a finite temperature, T_{BKT}, [12,13] characterized by a universal jump in the spin-wave stiffness (or helicity), ρ, of the system at T_{BKT} [14–16]. At low temperature, $T < T_{BKT}$, the correlation function, $C^{\alpha\alpha}$ (With $\alpha = x, y$), presents an algebraic decay $C^{\alpha\alpha}(r) \sim r^{-\eta}$. On the other hand, in the high temperature phase, the correlation function decays exponentially, $C^{\alpha\alpha} \sim e^{-ar}$. The situation for the diluted version of the model, when nonmagnetic disorder is included [17–21,23], is not clear.

The 2d model on a square lattice with nearest-neighbor exchange interaction undergoes a percolation transition upon dilution [24]. For the case of bond dilution, the transition occurs at the non-magnetic concentration $x_c^{bond} = 1/2$. For site dilution the percolation threshold is at $x_c^{site} \simeq 0.41$ [17].

Under the point of view of the transport phenomenon in two dimensions, the *XXZ* model is gapless. Sentef et al. [25] analyzed the spin transport in the easy-axis Heisenberg anti-ferromagnetic model in two and three dimensions, at $T=0$. Damle and Sachdev [26] treated the two-dimensional case using the non-linear sigma model in the gapped phase. Pires and Lima treated the two-dimensional easy plane Heisenberg antiferromagnetic model [27–29]. Lima [30] studied the case of the Heisenberg antiferromagnetic model in two dimensions with Dzyaloshinskii–Moriya interaction. Chen et al. [31] analyzed the effect of spatial and spin anisotropy on spin conductivity for the $S=1/2$ Heisenberg model

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on a square lattice. Within a self consistent harmonic approximation it is found that the *XXZ* model has a *BKT* transition. Upon site dilution the transition is extinguished at $x_s = 0.28$ [32], far below the percolation threshold x_c^{site}. On the other hand Sandvik [33] made a very careful quantum Monte Carlo simulation of the model at x_c^{site}. He found that the system has a transition which is compatible with a *BKT* transition. Costa et al. [32] made a quantum Monte Carlo simulation exploring the range $[0 \le x \le x_c^s]$. They followed the transition finding that it is possible that can change its character from *BKT* to another class of universality that they were not able to describe in detail.

A connection of the model with superconductivity and superfluidity can be done through the Ginzburg–Landau (*GL*) theory for temperatures below T_{BKT} (see for example Refs. [34–37]). The symmetric and broken phases in the spin model correspond to the superconducting (superfluid) and Coulomb (normal fluid) phases respectively in the *GL* approach. The key quantity to characterize the phase transition is the stiffness (or helicity) which is a response of the system to a twist of the spins along a specific direction. The stiffness is finite in the low temperature phase decaying to zero at T_{BKT}. The aim of this paper is to study the transport properties of the site diluted *XXZ* model in two dimensions as a function of the dilution x. Dilution corresponds to introduce defects in the system. Besides studying the interesting properties of spin transport we expect that it can give us a clue about the critical behavior of the system. This work is divided in the following way. In Section 2 we develop the analytical tools to obtain the transport properties of the model in the self consistent harmonic approximation (*SCHA*) [38–42]. In Section 3 we obtain the behavior of the conductivity, $\sigma^{reg}(\omega)$, as a function of the dilution x and the Drude weight, D_S. The last section is dedicated to our conclusions and final remarks.

2. Spin transport

The model we are interested in is defined by the following Hamiltonian:

$$\mathcal{H} = -J\sum_{\langle i,j\rangle}\varepsilon_i\varepsilon_j(S_i^xS_j^x + S_i^yS_j^y). \tag{1}$$

We take here $S=1$, $\langle i,j\rangle$ stands for the sum over nearest-neighbor and ε_i assume values 1,0 for magnetic or non-magnetic sites respectively. Sites are occupied with a probability distribution

$$\mathcal{P}[\varepsilon_n] = \prod_n P(\varepsilon_n),$$

$$P(\varepsilon_n) = [p\delta(\varepsilon_n - 1) + (1-p)\delta(\varepsilon_n)], \tag{2}$$

where p is the concentration of magnetic sites. We use the self consistent harmonic approximation [38–42] to determine the regular part of the spin conductivity and the Drude weight. A spin current appears if there is a gradient of magnetic field $\mathbf{B}$ through the system. It plays the role of a chemical potential for spins. One connect a low-dimensional magnet with two bulk ferromagnets. They act as reservoirs for spins [43]. One has a spin current if there is a difference, $\Delta\mathbf{B}$, between the magnetic fields at the two ends of the sample. As we are interested in calculating the longitudinal spin conductivity, we will add an external space and time-dependent magnetic field, $B(x,t)$, applied along the z-direction to the Hamiltonian (1). In the Kubo formalism [25,27,44] the spin conductivity is given by

$$\sigma(\omega) = \lim_{\vec{q}\to 0}\frac{\langle\mathcal{K}\rangle + \Lambda(\vec{q},\omega)}{i(\omega + i0^+)}, \tag{3}$$

where

$$\langle\mathcal{K}\rangle = \frac{J}{\hbar N}\sum_n \varepsilon_n\varepsilon_{n+x}\langle S_n^+S_{n+x}^- + S_n^-S_{n+x}^+\rangle. \tag{4}$$

S_n^+ (S_n^-) is a creation (annihilation) spin operator, $n+x$ is the nearest-neighbor site of site n in the positive x-direction and $\Lambda(\vec{q},\omega)$ is the current–current correlation function defined as

$$\Lambda(\vec{q},\omega) = \frac{i}{\hbar N}\int_0^\infty dt\, e^{i\omega t}\langle[\mathcal{J}(\vec{q},t),\mathcal{J}(-\vec{q},0)]\rangle. \tag{5}$$

$\Lambda(\vec{q},\omega + i0^+)$ is analytic in the upper half of the complex plane and extrapolation along the imaginary axis can be reliably done. Continuity equation for the lattice allows us to write the discrete version of the current as

$$\mathcal{J}_{n+x} - \mathcal{J}_n = -\frac{\partial S_n^z}{\partial t}. \tag{6}$$

The Heisenberg equation of motion $\dot{S}_n^z = i[\mathcal{H}, S_n^z]$ can be used with Eq. (6) to obtain

$$\mathcal{J} = \sum_n \mathcal{J}_{n,n+x} = \frac{iJ}{2}\sum_n \varepsilon_n\varepsilon_{n+x}(S_n^+S_{n+x}^- - S_n^-S_{n+x}^+). \tag{7}$$

Here we have assumed a magnetic field gradient along the x-direction. The real part of $\sigma(\omega)$, $\sigma'(\omega)$, can be written in a standard form as [45]

$$\sigma'(\omega) = \sigma_0(\omega) + \sigma^{reg}(\omega), \tag{8}$$

where $\sigma_0(\omega)$ is the *d.c.* contribution given by $\sigma_0(\omega) = D_S\delta(\omega)$, here D_S is Drude's weight

$$D_S = \pi[\langle\mathcal{K}\rangle + \Lambda'(\vec{q}=0,\omega\to\vec{0})]. \tag{9}$$

$\sigma^{reg}(\omega)$, the regular part of $\sigma'(\omega)$, is given by [45]

$$\sigma^{reg}(\omega) = \frac{\Lambda''(\vec{q}=0,\omega)}{\omega}. \tag{10}$$

It represents the continuum contribution to the conductivity. The Drude's weight measures the ability of the system to sustain a current without dissipation. In Eqs. (9) and (10), Λ' and Λ'' stand for the real and imaginary part of Λ respectively. We expect that at the percolation threshold both $\sigma^{reg}(\omega)$ and D_S should go to zero. We expect that anomalies in the critical behavior of the model should appear in those quantities.

3. Self consistent Harmonic approximation

The *SCHA* was originally proposed by Pokrovsky and Uimin to study the 2d classical planar rotator model [38]. Later, Minnhagen [5] pointed out that the *SCHA* overestimate the transition temperature because it did not take into account vortex fluctuations. He suggested a way to improve the thermodynamic described by this method by replacing the coupling constant, J, of the model by a renormalized, $J(T)$. This procedure leads to a better estimate of T_{BKT}. For example, it describes correctly the transition of the 1d quantum sine-Gordon model [46]. The reason is that it is equivalent to a renormalization group analysis in the one loop approach [46]. The approximation was successfully used in several other models [47]. Menezes et al. [39] extended the method to the classical *XY* model and Pires [40] applied it to its quantum version.

There is an extensive literature describing the *SCHA* [38–42], for this reason we will only sketch the main steps leading to the self consistent equations. Writing the spin components in the Villain representation [48]:

$$S_n^+ = e^{i\phi_n}\sqrt{\left(S+\frac{1}{2}\right)^2 - \left(S_n^z+\frac{1}{2}\right)^2}$$

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