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Doping effects in low dimensional antiferromagnets

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Abstract

The study of impurities in low-dimensional antiferromagnets has been a very active field in magnetism ever since the discovery of high-temperature superconductivity. One of the most dramatic effects is the appearance of large Knight shifts in a long range around non-magnetic impurities in an antiferromagnetic background. The dependence of the Knight shifts on distance and temperature visualizes the correlations in the system. In this work, we consider the Knight shifts around a single vacancy in the one- and two-dimensional Heisenberg model.

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Keywords: Low-dimensional antiferromagnets; Impurities; Spin chains

Doping and impurity effects in low-dimensional quantum antiferromagnets remain of strong interest in the condensed matter physics community, spurred by high-T_c superconductivity and other exotic effects in those systems. One of the most basic questions to ask is how an antiferromagnetic systems responds to an uniform applied magnetic field and how this response is changed in the presence of impurities. This question will be answered in detail for a two-dimensional (2D) spin-$\frac{1}{2}$ Heisenberg model. The results will then be compared to the one-dimensional spin-chain model which does not order at low temperatures.

Let us first consider a generic antiferromagnet, i.e. a collection of spins of size S which are assumed to order antiferromagnetically at low temperatures. This implies two sublattices A and B with long-range correlations throughout the lattice at low temperatures. The magnetic moments are correlated in parallel on the same sublattice, but antiparallel to the other sublattice. The size of the order parameter may be reduced by temperature or quantum fluctuations, but it is assumed to be non-zero. The effect of an applied magnetic field B can be intuitively understood as described by standard textbooks [1]. If the field is perpendicular to the order (transverse field), all spins can tilt slightly towards the field as shown in Fig. 1. A uniform magnetization is induced in the entire sample with a finite magnetic susceptibility $\chi = \partial m/\partial B = -\partial^2 F/\partial B^2$ at low temperatures. Note that if the field was applied parallel to the antiferromagnetic order, the response would be very small, since it costs more energy to induce a longitudinal magnetization. In an isotropic antiferromagnet, the order is therefore always aligned transverse to the field as shown in Fig. 1. At non-zero temperatures, spin-waves become excited, which can be polarized with the field. Therefore, the susceptibility increases with increasing temperature in the ordered phase. On the other hand, at very high temperatures in the non-ordered phase the susceptibility is well described by the Curie–Weiss-law $S(S+1)/3(T+\Theta)$, i.e. decreasing with temperature. The typical susceptibility of an antiferromagnet therefore shows a broad correlation maximum as shown in Fig. 2. Even in antiferromagnetic models which do not order at low temperatures this correlation maximum is well established, as for example in the spin-$\frac{1}{2}$ chain [2]. In this system the entangled quantum state gives rise to exotic effects such

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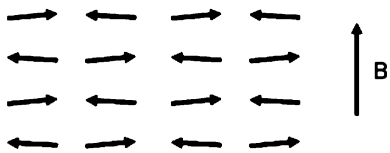

Fig. 1. The effect of a magnetic field B on a generic antiferromagnet.

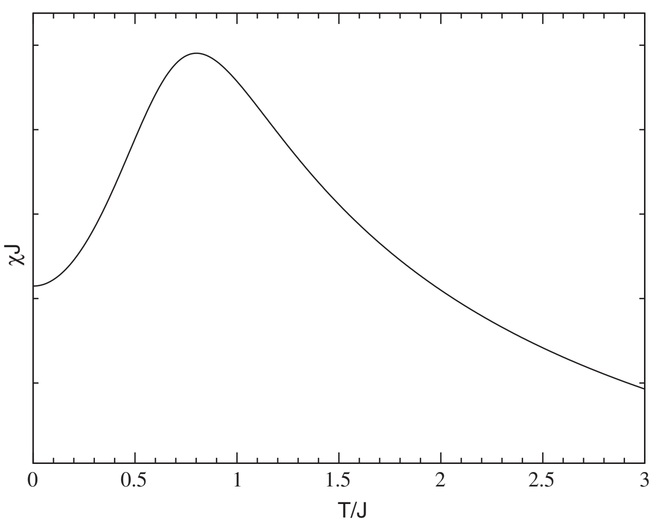

Fig. 2. Generic magnetic susceptibility for an antiferromagnet.

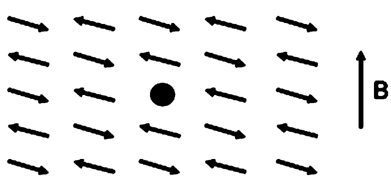

Fig. 3. The effect of a magnetic field B on an antiferromagnet with one single impurity (vacancy).

as a diverging derivative of the susceptibility with respect to T as $T \to 0$ [3].

We will now consider what happens to the individual spins when a vacancy is introduced into the antiferromagnetic order on sublattice B as shown in Fig. 3. Because of the antiferromagnetic order all spins on sublattice A form one large magnetic moment of size $SN/2$, while all spins on sublattice B amount to a magnetic moment of $S(N/2-1)$. The total system has, therefore, an effective net classical moment of size S which can align with the magnetic field, following a Curie-law with diverging susceptibility $S^2/3T$. This means that *all* spins on the sublattice A have a diverging susceptibility of $S^2/3T$ and all spins on sublattice B have a negative diverging susceptibility of $-S^2/3T$. This alternating Curie-type response is much larger than the uniform canting of the spins at low temperatures discussed above. One single impurity is therefore sufficient to induce an antiferromagnetic longitudinal order throughout the lattice in the presence of a magnetic field. So far we have neglected that in a quantum antiferromagnet the order parameter m is reduced by quantum fluctuations ($m=1$ represents the maximum alignment of all spins on the respective sublattices). Since the induced longitudinal order stems from the existing transverse order in the system, it must also be proportional to $mS^2/3T$ ($m\sim 80\%$ for the spin-$\frac{1}{2}$ Heisenberg AF on a 3D cubic lattice, and $m\sim 60\%$ on the 2D square lattice). Therefore, we can write approximately for the local response around an impurity, according to this intuitive picture

$$\chi(\mathbf{r}) = \chi_0 + (-1)^{r_x+r_y+1} m\,\frac{S^2}{3T}, \tag{1}$$

where χ_0 is the susceptibility per site of the pure system. The induced response is alternating (Fig. 3) while the uniform response remains largely unchanged (Fig. 1).

We will now test this picture for the 2D spin-$\frac{1}{2}$ Heisenberg model,

$$H = J\sum_{\langle i,j\rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \tag{2}$$

where $\langle i,j\rangle$ denotes nearest-neighbor sites on a periodic square lattice. This model is known to exhibit antiferromagnetic order as $T\to 0$. However, for any finite temperature the order is destroyed by quantum fluctuations. Among the ordered antiferromagnets, this model is therefore at the extreme borderline to a quantum entangled state. The quantum Monte Carlo program we developed uses the loop algorithm in a single cluster variety implemented in continuous time [4–7], which gives efficient and fast updates even at very low temperatures.

According to Eq. (1) the local response around a static vacancy

$$\chi(\mathbf{r}) = \beta \sum_i \langle S_i^z S_{\mathbf{r}}^z \rangle \tag{3}$$

can be separated into a sum of uniform and staggered parts on the lattice

$$\chi(\mathbf{r}) = \chi_{\mathrm{uni}}(\mathbf{r}) + (-1)^{r_x+r_y}\chi_{\mathrm{stag}}(\mathbf{r}), \tag{4}$$

the amplitudes of which are both slowly varying on the scale of one lattice spacing. In order to extract those two components we numerically extrapolate the data on the even sublattice to the odd sublattice and vice versa and define

$$\chi_{\mathrm{uni}}(\mathbf{r}) = \frac{\chi_{\mathrm{even}}(\mathbf{r}) + \chi_{\mathrm{odd}}(\mathbf{r})}{2}, \tag{5}$$

$$\chi_{\mathrm{stag}}(\mathbf{r}) = \frac{\chi_{\mathrm{even}}(\mathbf{r}) - \chi_{\mathrm{odd}}(\mathbf{r})}{2}. \tag{6}$$

The results for the staggered and uniform parts are shown in Figs. 4 and 5 for $T = 0.05\,\mathrm{J}$. The uniform part drops off very fast to the limiting value χ_0, but is strongly enhanced around the impurity. The staggered part also approaches a limiting value $\chi_\infty \sim 0.6\ (S^2/3T)$, which has the expected Curie-behavior as shown in Fig. 6 in agreement with $m\sim 0.6$ for the 2D Heisenberg model [8,9]. However, a broad peak around the impurity remains, which appears to be largely temperature independent. Therefore, Eq. (1) appears to be indeed valid for longer distances from the impurity, while for shorter distances quantum effects dominate. We expect that this picture becomes more and more accurate for larger spin models in higher dimensions. Our simulations for the 2D model are in full agreement with previous calculations, where the impurity susceptibility of the entire system has been considered [10–17]. For more details on the effect of more than one impurity, see Ref. [18].

We now wish to compare the situation to a model which does not order at low temperatures, such as the 1D spin-$\frac{1}{2}$ Heisenberg model. In this case, vacancies cut the chain, so that we need to consider a semi-infinite chain. This problem has been considered before [19], with some surprising results. A large alternating response is also induced by the impurity, but this *increases* with the distance from the edge. Finite temperatures, finite fields, or finite system sizes will limit the range of the alternating part, but generally the maximum alternating response is not closest to the impurity site. A typical response is shown in Fig. 7 for $T = 0.05$. It is clear that such a complicated pattern is an indication of a collective state in this quantum many body system, which gives some indication of the nature of the valence bond state [20].

In conclusion we have analyzed the local response to a uniform magnetic field in low-dimensional spin-$\frac{1}{2}$ antiferromagnets with one vacancy. For the 2D model an intuitive picture of a long-range antiferromagnetic order describes the results well far away from the impurity site. Only the more local enhancement is specific to the model and must be attributed to quantum effects or corrections from spin-wave theory. We therefore can argue that the local response is always accurately described by Eq. (1) for larger distances from a vacancy in *any* ordered antiferromagnet, where m is the order parameter, which typically depends on spin, dimension and temperature. Therefore, a single impurity induces a large Curie-divergent alternating

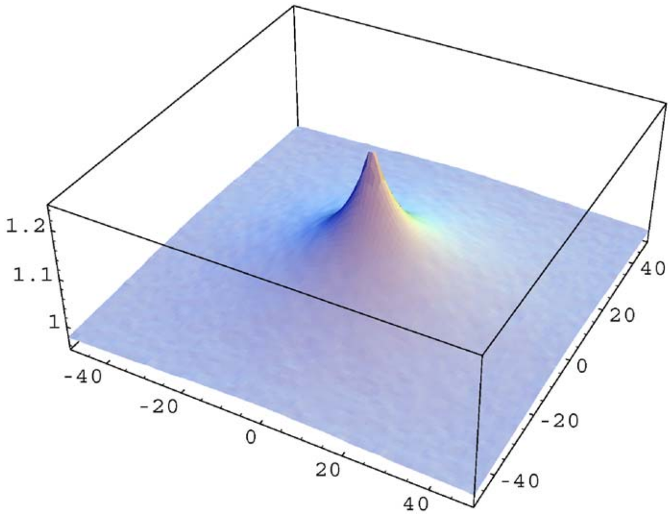

Fig. 4. (Color online) $\chi_{\text{stag}}(\mathbf{r})$ for $T = 0.05\,\text{J}$.

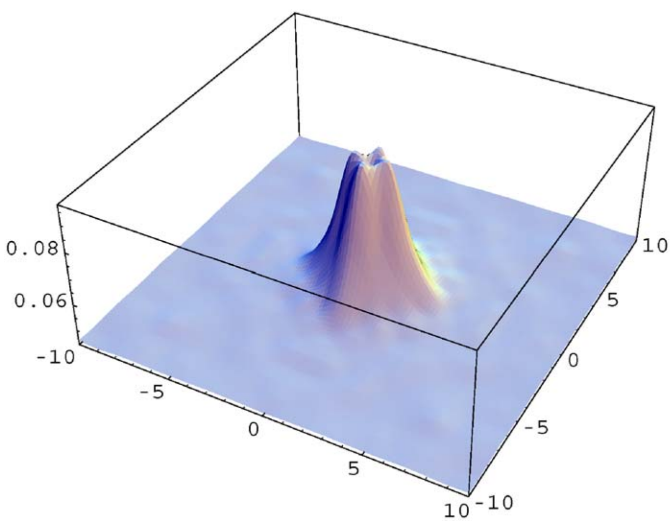

Fig. 5. (Color online) $\chi_{\text{uni}}(\mathbf{r})$ for $T = 0.05\,\text{J}$.

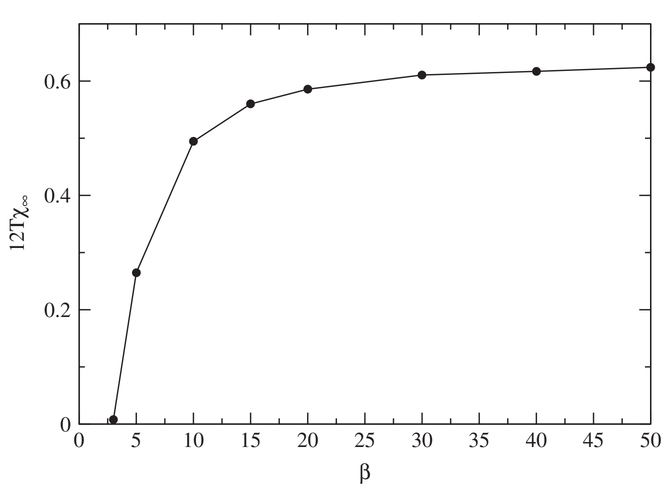

Fig. 6. The ratio $12T\chi_\infty$ as a function of $\beta = 1/T$.

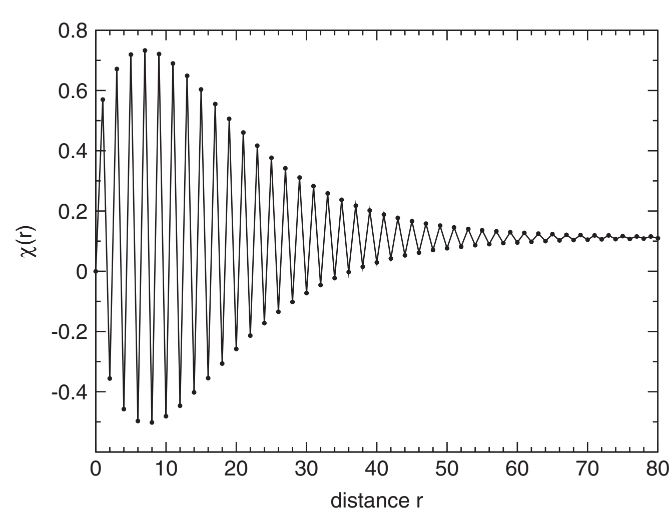

Fig. 7. The local response for a semi infinite chain at $T = 0.05\,\text{J}$.

response throughout an ordered antiferromagnet, if a field is applied transverse to the underlying magnetic order (this is automatically the case in an isotropic model). The response in the immediate vicinity is specific to the model, but can sometimes also be intuitively understood, e.g. by a valence bond basis [20]. The situation is quite different for the 1D quantum antiferromagnet, where strongly entangled quantum states dominate the picture.

Our results will have direct consequences on NMR and μSR experiments on doped antiferromagnets [21–24]. For the one-dimensional case the exotic boundary effects have already been confirmed, which are manifest through NMR satellites with a characteristic $1/\sqrt{T}$ dependence [24]. For ordered antiferromagnets it is important to distinguish between the ordered sublattice magnetization [25] and the field induced staggered magnetization, which we have described here. The field induced effects should show a more dramatic Curie-like temperature dependence and are assumed to be perpendicular to the sublattice magnetization.

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