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Interaction effects between impurities in low-dimensional spin-(1/2) antiferromagnets

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Abstract. – We are considering the interplay between several non-magnetic impurities in the spin-(1/2) Heisenberg antiferromagnet in chains, ladders and planes by introducing static vacancies in numerical quantum Monte Carlo simulations. The effective potential between two and more impurities is accurately determined, which gives a direct measure of the quantum correlations in the systems. Large effective interaction potentials are an indication of strong quantum correlations in the system and reflect the detailed nature of the valence bond ground states. In two-dimensions (2D) the interactions are smaller, but can still be analyzed in terms of valence bonds.

Introduction. – The interplay between impurities in antiferromagnetic backgrounds has become an important topic ever since the discovery of high-temperature superconductivity. The interaction energy between mobile holes has been examined with a variety of numerical and analytical methods for t-J and Hubbard models in order to get a better insight into the pairing mechanism in the HiT_c compounds [1–4]. Equally interesting is the effect of static impurities [5–9] which, for example, are known to induce spin-(1/2) degrees in ladders, that interact to form gapless excitations in otherwise gapped systems [10,11]. For static vacancies one of the first studies was performed by Bulut *et al.* with linear spin-wave approximation and numerics on small lattices [5], establishing a nearest-neighbor attraction and an interesting enhancement of the local quantum correlations.

We are now considering several static holes (vacancies) in low-dimensional antiferromagnets like chains, ladders and planes on larger lattices, in order to calculate their impurity and interaction energies in the limit of zero temperature. The energies are changed because nearest-neighbor correlations $\langle \boldsymbol{S}_i \cdot \boldsymbol{S}_j \rangle$ are altered around the vacancies which in turn visualize the quantum correlations on the lattice. Therefore the interaction energy between two or more impurities gives direct information on the quantum correlations by showing the underlying local valence bond order as will be explained for a variety of configurations in the antiferromagnetic spin-(1/2) Heisenberg model $H = J \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j$, where $\langle i, j \rangle$ denotes nearest-neighbor sites on chain, ladder and square lattices.

In order to determine impurity contributions to the total energy and the effective potentials between vacancies, we have to sum up all bond strengths in the system and subtract the

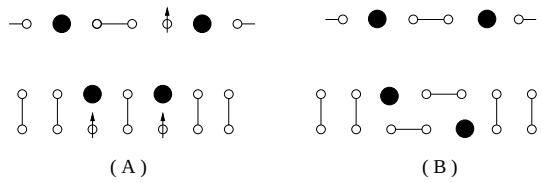

Fig. 1 – Different configurations of valence bonds around impurities. In cases A it is not possible to construct a simple valence bond state around the impurities, so the energy cost is higher. In the cases B the energy is lowered because quantum correlations on sites between the impurities are enhanced by the valence bonds as drawn.

reference energy of a pure system. Since it is necessary to subtract two large extensive quantities, the energies E for each configuration must be determined to at least six significant digits in our case. For practical purposes this limits the system sizes for determining the impurity energies to a periodic 16×16 lattice for the 2D geometry. The quantum Monte Carlo program we developed uses the loop algorithm in a single cluster variety implemented in continuous time [12–15], which gives efficient and fast updates even at very low temperatures. From now on all temperatures and energies are given in units of $J = 1$.

In order to understand the meaning of the interaction energy between impurities, let us first consider the extreme limit of the absence of all quantum fluctuations like in the Ising model, where the ground state is characterized by a purely classical Néel order. Substitutional impurities remove antiferromagnetic bonds, but do not change the ordered ground state and cannot feel an effective potential between each other except for a nearest-neighbor attraction, since more antiferromagnetic bonds are present when impurities are placed on neighboring sites. However, in systems with an entangled quantum ground state there is a possibility that impurities can have an effective potential over several lattice sites, since the quantum correlations are strongly altered by the impurities (while classical order is not). Such quantum correlated systems can often be best described in terms of a resonating valence bond basis or a valence bond solid. In that case, there is a higher energy cost if impurities are placed in such a way that the valence bonds (singlets) cannot be accommodated between the vacancy sites, while the effective potential may be attractive if resonating valence bonds fit exactly between the impurities. In effect the vacancies prune the possible singlet formation analogous to the ideas of Martins *et al.* [16,17], where the antiferromagnetic order around single impurities was discussed. Figure 1 shows typical examples for attractive and repulsive configurations in chains and ladders, for which resonating valence bonds form a good description of the systems. The effective potential between vacancies is therefore a direct indication both of the configuration and the amount of quantum correlations in the system as compared to a classical Néel state.

Vacancies in spin-chains. – In the one-dimensional case, vacancies simply cut the infinite chain, so that the impurity interaction potential can easily be determined from the ground-state energy of the finite segment between the impurities. Finite Heisenberg spin chains are extremely well studied so that the interaction potential can be calculated analytically up to higher-order corrections. It is useful to approximate the ground-state energy $E_{\rm gs}(L)$ for a finite chain of length L in the form

$$E_{\rm gs}(L) = \epsilon_0 L + E_s + \frac{b}{L} + \mathcal{O}\left(\frac{1}{L\ln(L)}\right), \tag{1}$$

where $\epsilon_0 = 1/4 - \ln 2$ is the thermodynamic limit of the energy per site and $E_s = \frac{\pi-1}{4} - \frac{\ln 2}{2} \approx 0.1888$ is the surface energy for open boundary conditions [18]. The single-impurity energy

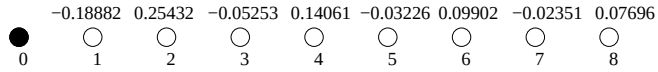

Fig. 2 – The exact impurity-impurity interactions in the 1D lattice.

is given by the difference of total energy of the pure system E_0 and of a system with one impurity E_1

$$\Delta E = E_1 - E_0 = E_s - \epsilon_0 \approx 0.632. \tag{2}$$

This impurity energy ΔE is smaller than the energy cost of two missing links $-2\epsilon_0 \approx 0.8863$, because the quantum correlations are changed in the ground state (which would not be the case in an Ising-like system). The effective impurity-impurity potential $U(x)$ can be extracted by comparing the total energy $E(x)$ in a given configuration to a reference energy $E(\infty)$, corresponding to two vacancies very far apart. Equivalently, we can also define the reference energy as the extra energy cost of two single impurities $E(\infty) = E_0 + 2(E_1 - E_0)$. Accordingly, the surface energy and energy per site cancel, and the leading contribution comes from the $1/L$ term in eq. (1), which is known from conformal field theory to be $b = -\pi^2/48$ for open chains with even number of sites [19]. However, for an odd number of sites the ground state quantum numbers correspond to an excited state in terms of the field theory [20] and for odd open chains we have [21] $b = 5\pi^2/48$. We therefore find

$$U(x) = E(x) - E(\infty) \approx (-1)^x \frac{\pi^2}{16x} + \frac{\pi^2}{24x}, \tag{3}$$

which is an alternating potential with a relatively large magnitude and a slow power law decay in agreement with the intuitive picture in fig. 1. The results for shorter distances can easily be calculated exactly and are shown in fig. 2, which only slowly approach eq. (3) because of the logarithmic corrections in eq. (1). Interestingly, the nearest-neighbor attraction is not very large, which comes from the fact that not very many quantum valence bonds are enhanced by this configuration compared to two isolated impurities. On the other hand, the repulsion for $U(2)$ is even stronger in magnitude since this placement of vacancies disrupts the valence bond configuration very strongly. This is generally true for an odd number of sites between the vacancies as is intuitively clear from fig. 2.

Vacancies in spin-ladders. – An equally interesting example of a quantum-dominated ground state is the two-leg ladder which can locally be described by a valence bond solid but with short-range correlations due to an energy gap. Placing a single impurity into this system is already rather disruptive to the ground state, which is reflected by the relatively high energy cost of $\Delta E \approx 1.215$. However, this energy is almost completely accounted for by the missing energy bonds along the legs $\epsilon_{\text{leg}} \approx 0.350$ and across the rungs $\epsilon_{\text{rung}} \approx 0.455$, as if the ground-state configuration of the entire system was not changed except for the local

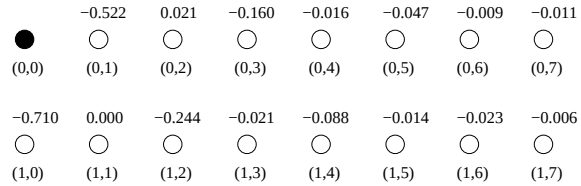

Fig. 3 – Potential $U(x, y)$ between static holes for a two-leg ladder of size 2×40 with $\beta = 15$ calculated as $E_{(x,y)} - E_{2,20}$.

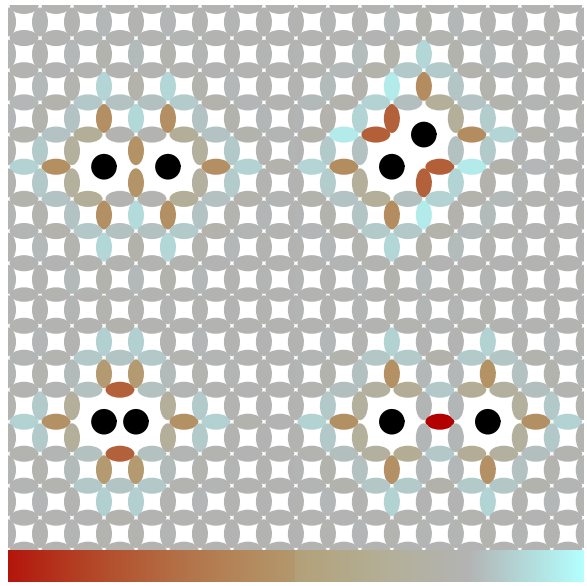

Fig. 4 – (Color online) Different configurations of impurities in the 2D Heisenberg antiferromagnet and the corresponding bond strengths on a scale ranging from -0.4365 to -0.312. In the upper two cases the valence bonds are disrupted in a relatively large area around the vacancies, so that the energy cost is higher. In the last case the energy is lowered because quantum correlations on sites between the impurities are enhanced.

extraction of the missing bonds. The numerical results for the effective impurity-impurity potential of a 2×40 ladder system are presented in fig. 3.

The strongest potential is found for the nearest-neighbor attraction, which is stronger across the rungs than along the legs, in accordance with the different energies per bond $\epsilon_{\text{leg}} < \epsilon_{\text{rung}}$. For larger distances a staggered potential can be observed, which is however predominantly negative. This means that in most cases the valence bond state can be partially repaired between two close vacancies, even for two impurities on the same sublattice. Interestingly, the zig-zag pattern of attractive energies along the sites on the opposite sublattice $(1,0),(0,1),(1,2),(0,3)...$ fits well to an exponential decay $U(r) \sim -1.05\exp[-0.632r]$ with geometrical distance r. This means that the potential decay length $\xi_U \sim 1.58$ is almost exactly half of the decay length for correlations $\xi \sim 3.19$ [22] or for effective spin interactions $\xi \sim 3.1$ [10]. The overall magnitude of the potential is relatively large as expected for a system with strong quantum correlations, but it remains short-ranged.

Vacancies in the 2D Heisenberg antiferromagnet. – In contrast to chains and ladders the 2D Heisenberg antiferromagnet is not dominated by strong quantum correlations. Instead it is believed to be well described by spin waves on top of a Néel ordered state. However, some valence bond character may still remain, especially on shorter distances, which will be revealed by the study of the impurity-impurity interactions. As argued above, a classical antiferromagnetic order does not imply any interaction energies, so that the impurity-impurity potential will give information about the magnitude and nature of the remaining valence bond character in the 2D antiferromagnet.

Indeed we find a pronounced change of the correlation strengths $\langle \boldsymbol{S}_i \cdot \boldsymbol{S}_j \rangle$ of the nearest-neighbor bonds as is shown for some typical arrangements in fig. 4 at low temperatures from

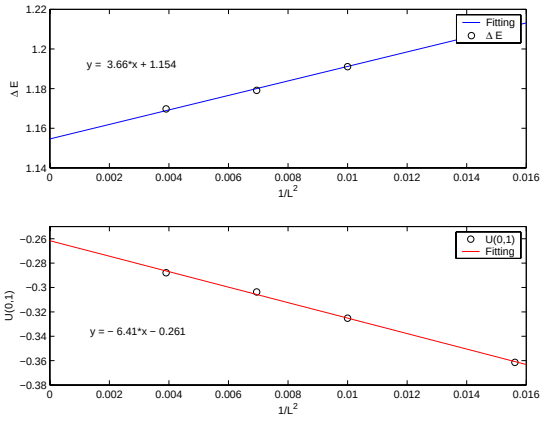

Fig. 5

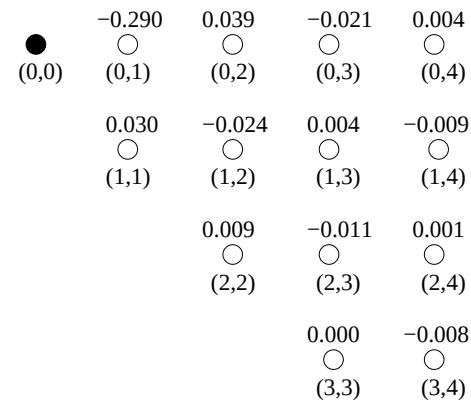

Fig. 6

Fig. 5 – (Color online) The finite-size scaling of ΔE and $U(0,1)$ in an $L \times L$ lattice demonstrating the $1/L^2$ scaling for impurity quantities. The size of the symbols corresponds approximately to the error of 0.002.

Fig. 6 – Potential $U(x,y)$ between static holes in a 2D antiferromagnet on a 16×16 lattice.

our numerical simulations. A minimum value of -0.75 would correspond to a singlet and $\epsilon_0 \approx -0.3347$ is the bulk value. The valence bond character closest to the impurities is always enhanced [16, 17], but this can lead to a weakening of other bonds. The sum of all bond strengths gives the total energy and there may be a net energy cost (or gain), depending on the configuration. For example, if a vacancy is placed at $(0,0)$ and a second vacancy at $(1,1)$ or $(0,2)$, the valence bond order is disturbed locally so that we see a net energy cost. For a second vacancy at $(0,3)$, on the other hand, the valence bond between the impurities is so strongly enhanced as shown in fig. 4 that this configuration is energetically relatively favorable. All simulations of fig. 4 were done on a 16×16 lattice at $\beta J = 30$, but are shown in one single plot for convenience.

One vacancy. For the single-impurity case, we find an energy cost of $\Delta E = E_1 - E_0 \approx 1.154$ which is smaller than the energy cost of removing four bonds $\Delta E + 4\epsilon_0 \approx -0.18$, where $\epsilon_0 \approx -0.3347$. Those results compare well with linear spin-wave estimates of Bulut *et al.*'s [5] where it was observed that large lattices are necessary for convergence, which is an indication that the system is affected by the impurity over relatively large distances. In fig. 5 the scaling behavior for the most important quantities is shown, indicating that ΔE has converged to almost 99% for a 16×16 lattice. Typically, impurity quantities converge to the thermodynamic limit with $1/L^2$ while ϵ_0 converges with $1/L^3$ on an $L \times L$ lattice [5].

Two vacancies. In order to determine the impurity-impurity potential we place the first vacancy at $(0,0)$ and a second one in several different positions (x,y). The total energy of the system $E_{(x,y)}$ is then calculated numerically in each case. According to eq. (3), we define the effective impurity-impurity potential $U(x,y) = E_{(x,y)} - E_{(\infty,\infty)}$. For the reference energy it turns out that a vacancy at maximum distance is already a perfect approximation within numerical accuracy, *i.e.* $E_{(\infty,\infty)} \approx E_{(8,8)}$, which can also be determined with a lower statistical error than the extra energy cost of two single impurities $E_{(\infty,\infty)} = E_0 + 2(E_1 - E_0)$.

Figure 6 shows the results of our numerical analysis for $U(x,y)$ within our statistical error of ± 0.002 on a 16×16 lattice at $T = J/30$. Not surprisingly the dominant contribution is given by an attractive nearest-neighbor interaction, which is due to the fact that one more

TABLE I – *The potential for three vacancies at* $(0,0)$*,* (x_1,y_1) *and* (x_2,y_2) *compared to the sum of two body potentials* $U_{\rm corr} = U(x_1,y_1;x_2,y_2) - U(x_1,y_1) - U(x_2,y_2) - U(x_1-x_2,y_1-y_2)$ *in a* 16×16 *lattice for* $\beta J = 30$*. The last digit is uncertain.*

$(x_1,y_1),(x_2,y_2)$	$U(x_1,y_1;x_2,y_2)$	$U_{\rm corr}$
$(0,1),(0,2)$	-0.573	-0.032
$(0,1),(1,0)$	-0.531	0.019
$(0,1),(0,3)$	-0.259	0.013
$(0,1),(1,2)$	-0.287	-0.003
$(0,1),(2,1)$	-0.268	0.007
$(1,1),(2,0)$	0.105	0.006
$(1,1),(2,2)$	0.066	-0.003
$(2,0),(2,2)$	0.084	-0.003
$(0,8),(8,8)$	0	0

antiferromagnetic bond is present for this configuration. This is comparable to the Ising model, but here the value for $U(0,1)$ is only about 80% of the average energy per bond ϵ_0, indicating that quantum correlations account for the difference of 20%. The numerically extrapolated binding energy of $U(0,1) = -0.261$ for an infinite system is in good agreement with the linear spin-wave theory (LSW) result [5] $U_{\rm LSW}(0,1) = -0.2666$.

The quantum correlations become even more evident for larger distances which show a staggered effective potential. As explained above, this staggered potential is not caused by a Néel antiferromagnetic order, but is an indication of how efficiently valence bonds can be arranged around the impurities as already shown in fig. 4. In particular, there is a higher energy cost when the second impurity is placed at $(0,2)$ or $(1,1)$, which are disruptive configurations for regular valence bond arrangements. If an impurity is placed at $(0,3)$ on the other hand, a valance bond can be formed very efficiently between the sites $(0,1)$ and $(0,2)$ so that in this case the enhanced quantum correlations lead to a gain in total energy and an effective attractive potential. Continuing in this way an effective staggered potential is formed. Although the potential is small, it is not necessarily short-ranged. The relatively slow scaling of $U(0,1)$ with system size and the fact that the bond strengths in fig. 4 are altered over a large area indicate that vacancies can affect the system over a long range. However, since the effective potential for distances larger than one is always much smaller than typical kinetic energies of mobile holes would be, it is unlikely that directly magnetically mediated impurity-impurity potentials could significantly contribute to the pairing mechanism in high-temperature superconductors except for nearest-neighbor interactions.

Three vacancies. If a third vacancy is now placed in the system, it will interact with the other two vacancies with the same mechanism as before, namely as a probe of which possible valence bonds have been pruned. This means that the three-body potential can in general not be written as a sum of two-body potentials. For comparison we introduce a three-body correction $U_{\rm corr}$ for impurities placed at $(0,0)$, (x_1,y_1) and (x_2,y_2):

$$U(x_1,y_1;x_2,y_2) = E_{x_1,y_1;x_2,y_2} - E_\infty = U(x_1,y_1) + U(x_2,y_2) + U(x_1-x_2,y_1-y_2) + U_{\rm corr}, \quad (4)$$

where E_∞ is the configuration energy of three impurities infinitely apart from each other. In our case we can approximate $E_\infty \approx E_{0,8;8,8}$. The correction term $U_{\rm corr}$ is a measure of how disruptive the total three-impurity configuration is. If, for example, the third impurity is placed on a valence bond that is strongly enhanced by the two first impurities combined, we expect an additional penalty. In table I the results for the most interesting configurations are shown. The dominant contribution comes again from the nearest-neighbor attraction, which is just a

trivial count of how many antiferromagnetic bonds are present. However, the correction $U_{\rm corr}$ is found to be of the same order as the longer-range potentials and other quantum corrections. Therefore, many-body effects are essential when describing the interaction. In particular, it is more efficient to place three vacancies in a line $(0,0),(0,1),(0,2)$ than placing them at an angle $(0,0),(0,1),(1,0)$, because valence bonds can form more efficiently along straight edges (note that we would get the opposite statement if there were no three-body correction $U_{\rm corr}$).

Conclusions. – In conclusion, we have analyzed the interplay of several vacancies in antiferromagnetic spin-chains, spin-ladders, and planes in the low-temperature limit. For chain and ladder systems large effective potentials can be found, which is a direct indication of their well-established strongly entangled ground states over long and short ranges, respectively. In the 2D case, a small effective potential between two static vacancies can be explained in terms of a small quantum valence bond character on top of the Néel order. The corresponding energies are of the order of 10-20% of one bond strength, which gives an indication of the size of the quantum corrections in this system. Despite the smallness of the potential, the bonds are affected over a long-range around the impurity. The potential is not a simple two-body effect, which is in agreement with the assumption that it originates from possible valence bond arrangements (and the pruning of them).

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