Staggered magnetization and entanglement enhancement by magnetic impurities in $S = 1/2$ spin chain

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We study the effects of a magnetic impurity on the behavior of a $S = 1/2$ spin chain. At $T = 0$, both with and without an applied uniform magnetic field, an oscillating magnetization appears, whose decay with the distance from the impurity is ruled by a power law. As a consequence, pairwise entanglement is either enhanced or quenched, depending on the distance of the spin pair with respect to the impurity and on the values of the magnetic field and the intensity of the impurity itself. This leads us to suggest that acting on such control parameters, an adiabatic manipulation of the entanglement distribution can be performed. The robustness of our results against temperature is checked, and suggestions about possible experimental applications are put forward.

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The prospect of quantum technology, i.e., the design and realization of quantum devices, is triggering an increasing interest in the manipulation of quantum systems in view of several applications, amongst which is quantum information processing [1]. Despite the large variety of experimental proposals, the relevant properties of most of such devices can be adequately described by a few classes of models. Quantum low-dimensional spin models constitute one such class: They may describe different physical systems and, at the same time, their Hamiltonian is simple enough to allow an easy recognition of the parameters responsible for specific effects, so that simple controls may be designed to drive focused manipulations. Sticking to strictly one-dimensional models, a possibility of manipulation is offered by the introduction of local impurities, either magnetic or not, which break the translational symmetry. In the last decade, several studies have been devoted to low-dimensional systems with inhomogeneities 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, revealing peculiar phenomena which occur in the vicinity of the impurity.

In this paper, we consider the less investigated case of magnetic impurities, which can couple both with neighboring spins and/or with external magnetic fields, offering a remarkable control flexibility. In particular, aimed at possible application in the realm of quantum computation, we consider a single impurity in the $S = 1/2$ XX chain in a transverse field in its quasi-long-range ordered phase. In the absence of impurity and due to the high symmetry of the exchange interaction, such model displays values of bipartite entanglement larger than those observed in less symmetric models 13. The impurity is modelled in terms of an additional field located at one precise site of the chain. We study the ground-state properties and thermodynamic behavior when the field and/or the magnetic strength of the impurity are varied.

At zero temperature, we find an infinite penetration depth for the effects of the magnetic impurity, namely it produces spatial modulations of the spin configuration which decay polynomially with the distance from the impurity itself. A staggered magnetization and an oscillating susceptibility result, as a most general consequence of translational symmetry breaking 14. One striking effect of the emergence of such spin structure is the local enhancement of pairwise entanglement: When no uniform field is applied, the concurrence 14, 15 of the spin-pair next to the impurity doubles with respect to the translational invariant case and, consequently, an entanglement re-distribution takes place all over the chain. With finite magnetic field, there always exists a most entangled spin pair, which can be moved along the chain by tuning either the field or the impurity strength. These parameters can thus play the role of ”knobs” for the manipulation of both the magnetic and the entanglement properties of the chain. Furthermore, as they appear in terms that commute with the Hamiltonian, adiabaticity is guaranteed while tuning their values. The essential features of the above picture, and in particular the possibility of selectively enhance pairwise entanglement, survive at finite temperature. This gives a concrete possibility to experimentally test our findings.

Let us consider the Hamiltonian

$$\mathcal{H} = -\sum_{n=-N}^{N-1} \left[ \frac{1}{2}(\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y) + h \sigma_n^z \right] + \alpha \sigma_0^z, \quad (1)$$

where $\sigma_n^\varepsilon (\varepsilon = x, y, z)$ are the the Pauli operators for the spin at site $n$, and periodic boundary conditions are assumed. A uniform magnetic field $H$ is applied along the quantization axis, which takes values such that $h \equiv g_\mu_B H/J \in [-1, 1]$: the exchange integral $J$ is set to unity throughout the paper. The magnetic impurity
is located at site 0 and represented by a local magnetic field \(\alpha\) [10]. As \(\mathcal{H}\) can describe several physical systems beyond the mere spins (e.g., atoms loaded in optical lattices), one may think of correspondingly several ways of introducing a localized defect. In general the impurity breaks the translational symmetry and as \(\alpha \to \infty\) it renders the system equivalent to an open-end chain.

The Hamiltonian (1) can be diagonalized by standard methods [17, 18], resulting in an energy band and in a localized level

\[
\mathcal{H} = \sum_k E_k g_k \sigma_k + E_{\alpha} g_\alpha \sigma_\alpha .
\]

Here, \(E_k = h - (\text{sgn} \alpha) \sqrt{1 + \alpha^2}\) is the energy of the localized state, while the corresponding fermion operator is a combination of the Jordan-Wigner ones \(\{c_n^\dagger\}\)

\[
g_\alpha = \sum_n \varphi_{n,\alpha} c_n^\dagger ; \quad \varphi_{n,\alpha} = -\sqrt{|\alpha| (\text{sgn} \alpha)} n (1 + \alpha^2)^{-1/2} e^{-|n|/\xi} ,
\]

with \(\xi^{-1} \equiv -\ln(\sqrt{1 - \alpha^2} - |\alpha|)\). Concerning the band, \(E_k = h - \cos \theta_k\) is the unperturbed dispersion relation \((\theta_k = \frac{2ck}{N}, k = -\frac{N}{2}, \ldots, \frac{N}{2} - 1)\), while

\[
g_k = \sum_n \varphi_{n,k} c_n^\dagger ; \quad \varphi_{n,k} = e^{i\theta_k n} - \frac{\alpha e^{i\theta_k |n|}}{i \sin |\theta_k| + \alpha} .
\]

The impurity is seen to produce i) the appearance of a discrete energy level (lying above or below the band depending on the sign of \(\alpha\), exponentially localized in space with a characteristic length \(\xi\); and ii) the distortion of the energy-band states, whose amplitudes, besides the plane wave term, contain a back-scattering contribution due to the defect. It is precisely the interference between these two terms that gives rise to the oscillating patterns discussed below in both the magnetization and the susceptibility.

Using the Wick’s theorem, we calculate one- and two-point correlation functions which, due to the lack of translational symmetry, cannot be expressed as Toeplitz determinants, so that their expressions become more and more involved with the relative site distance. We find:

\[
\langle \sigma_r^z \rangle = 1 - 2 \sum_{\eta \in \mathcal{F}} |\varphi_{r,\eta}|^2 , \quad (\sigma_r^x \sigma_{r+1}^x) = 2 \text{Re} \sum_{\eta \in \mathcal{F}} \varphi_{r,\eta}^* \varphi_{r+1,\eta} ,
\]

\[
\langle \sigma_r^x \sigma_{r}^{\pm} \rangle = 1 - 2 \sum_{\eta \in \mathcal{F}} (|\varphi_{r,\eta}|^2 + |\varphi_{s,\eta}|^2) + 4 \sum_{\{\eta,\nu\} \in \mathcal{F}, \eta \neq \nu} (|\varphi_{s,\eta}|^2 |\varphi_{r,\nu}|^2 - \varphi_{r,\eta}^* \varphi_{s,\eta}^* \varphi_{r,\nu}^* \varphi_{s,\nu})
\]

where \(\mathcal{F}\) is the set of filled states. Rotational symmetry gives \(\langle \sigma_r^x \rangle = \langle \sigma_r^y \rangle = 0\) and \(\langle \sigma_r^x \sigma_{r+1}^x \rangle = \langle \sigma_r^y \sigma_{r+1}^y \rangle\); moreover, reflection symmetry with respect to site 0 allows us to consider only \(r \geq 0\) in the following.

In the thermodynamic limit, the local magnetization at zero temperature takes the form

\[
\langle \sigma_r^z \rangle = \langle \sigma_r^z \rangle + \frac{2\alpha}{\pi} \int_0^{\theta_F} d\theta \frac{\alpha \sin(2r \theta) + \sin \theta \sin(2r \theta)}{\alpha^2 + \sin^2 \theta} ,
\]

with \(\theta_F \equiv \cos^{-1} h\) and where \(\langle \sigma_r^z \rangle = 1 - \frac{2\alpha}{\pi}\) gives the result without defect, \(\langle \sigma_r^z \rangle = -2|\varphi_{r,\eta}|^2\) is due to the localized state (this term is present only for \(\alpha > 0\), while the last term is due to the interference mechanism mentioned above. The essential finding embodied in Eq. (5) is the emergence of an oscillating magnetization in the vicinity of the impurity, as shown in Fig. 1.

Several works [2, 3, 4, 5, 6, 7, 8, 9, 10, 11] have evidenced that finite staggered moments are induced by open ends in antiferromagnetic spin chains and that the spatial decay of the related magnetization is ruled by the (bulk) correlation length of the infinite, translational invariant, system. Previous analysis, however, referred to spin chains in disordered phases, with exponentially decaying correlations, either because of the finite temperature or due the symmetry of the Hamiltonian itself, as in the case of the Haldane chains. On the contrary, our model is independent of the sign of the exchange coupling and, at \(T = 0\), it is in a quasi-long-range ordered phase with an infinite correlation length and a much slower (power law) decay of the correlation functions. The effects of the impurity are consequently felt by more distant spins along the chain. Indeed, there exists a precise analogy [10] between our model and the case of a one-dimensional fermionic system in the presence of one impurity, where Friedel oscillations occur [19]: for \(\alpha \gg 1\) and \(r \gg 1\) Eq. (6) gives the same \(\frac{1}{r}\) behavior predicted for the oscillations of the fermion density in a Luttinger liquid with a defect [20]. It is noteworthy that, at variance with the case of the XX chain with locally inhomogeneous exchange interaction [9], the presence of the magnetic impurity gives rise to Friedel-like oscillations even when no uniform field is present.

In general, for a fixed \(h\), the value of \(\alpha\) determines the absolute value of the local magnetization, while, independently of \(\alpha\), the field fixes the spatial periodicity \(p\) of the oscillations (see Fig. 1). In fact, we see that \(p\) coincides
with the period of the connected correlation functions of the translational-invariant model, i.e. $p = \frac{\pi}{\sqrt{2}}$. This behavior is understood by observing that the local switching-on of $\langle \sigma_{z}^{r} \rangle$ under the effect of the local field at site 0 is mediated by the generalized magnetic susceptibility, which in turns has the same spatial dependence of the correlation functions.

Let us now consider the local magnetic susceptibility. From Eq. (5), we get $\chi_{\tau}(\alpha, h) = 2/(\pi \sqrt{1 - h^2}) + \chi_{\tau}^{alt}(\alpha, h)$, where the alternating term is

$$
\chi_{\tau}^{alt}(\alpha, h) = -2\alpha \frac{\cos(2r\theta_F) + \sqrt{1 - h^2} \sin(2r\theta_F)}{\pi(1 + \alpha^2 - h^2)\sqrt{1 - h^2}} \quad (6)
$$

The superposition of a uniform term and a spatially oscillating one, is fully analogous with the results relative to the spin-$\frac{1}{2}$ Heisenberg antiferromagnetic chain with open ends \[3\] or bond impurities \[2\]. The alternating term survives throughout the chain with a spatial structure that, being $r$ an integer, follows peculiar, beating-like, patterns, depending on the value of $h$. When $h = 0$, one has $\chi_{\tau}(\alpha, 0) = \frac{2}{\pi} (1 - \frac{(1 - \alpha^2)}{1 + \alpha^2})$ meaning that, for $\alpha \gg 1$, odd-labelled spin increase their susceptibility up to the value $\frac{2}{\pi}$, while even-ones have zero susceptibility.

Noticeably, $\chi_{\tau}(\alpha, h)$ does not diverges at the critical point $h = 1$. In fact, while in the translational invariant model the susceptibility diverges as $(1 - h)^{-1/2}$ for $h \to 1$, we find here that in the same limit $\chi_{\tau}(\alpha, h) \approx \frac{2\sqrt{2(1-h)}}{\pi} \left( \frac{1+2r\alpha}{\alpha^2 + 2(1-h)} \right)$. As a consequence of the translational symmetry breaking, singularity is cancelled and all susceptibilities vanish at the critical point.

The spatial modulation of the magnetic susceptibility described in Eq. (6), offers a chance to selectively act on local spins. This possibility is at the hearth of the following discussion about local enhancement and possible transfer of entanglement.

As stated in the introduction, due to the high symmetry of its Hamiltonian, the XX model has a markedly entangled ground state, with next neighbor concurrences larger than those observed in less symmetric models \[13\]. Furthermore, the rotational invariance forces bipartite entanglement to be of antiparallel type \[22, 23\]. This property holds also when translational invariance is broken. This fact, together with the emergence of the staggered structure described above, suggests an enhancement of the nearest neighbor concurrences. This is shown to occur in Fig. 2 where $C_{12}$ and $C_{23}$ are displayed vs $h$, for different values of $\alpha$. In particular, at zero field and for large $\alpha$, $C_{12}$ is more than twice its value without defect, and a similar enhancement is observed in $C_{23}$ for two different values of $h$. In general, $C_{r,r+1}$ displays $r$ maxima, whose position in the $[-1,1]$ field interval is increasingly symmetric, with respect to the value $h = 0$, as $\alpha$ increases. The maximum values of $C_{r,r+1}$ are always larger than those attained for $\alpha = 0$, but the difference is smeread out with increasing $r$ (i.e., by moving far from the impurity). The highly non trivial behavior of $C_{r,r+1}$ with respect to $h$, $r$ and $\alpha$, is formally due to the interference phenomenon embodied in Eq. (6). Physically it is a consequence of an entanglement re-distribution, resulting from the constraints imposed by the monogamy inequality \[24, 25\] on a locally modulated spin-structure.

In particular, for $h = 0$ and independently of $\alpha$, the most entangled spin pair is the one adjacent to the impurity and the one-angle $r = 1 - \langle \sigma_{z}^{r} \rangle^2$, with $r \neq 0$, does not vary much with $r$ and it is substantially insensitive to $\alpha$. The observed alternating behaviour of $C_{r,r+1}$, which gets a larger or smaller value with respect to the translational invariant case according with $r$ being odd or even, respectively, can thus be interpreted as a consequence of the monogamy inequality. Furthermore, the difference between $C_{r,r+1}$ and $C_{r+1,r+2}$ increases with $\alpha$ and a sort of entanglement dimerization is observed for large impurity strength.

For $h \neq 0$, $C_{r,r+1}$ displays an increasingly complicated dependence on $h$ and $\alpha$, which gives rise to a sharp-cut mechanism of entanglement transfer for $h \lesssim 1$. In such case indeed, as shown in Fig. 3 for $h = 0.9$ and $0.99$, a most entangled spin pair is still detected at a distance from the impurity that increases with $h$. Hence, by varying either the defect strength or the magnetic field, one can drive the maximum of the concurrence along the chain, meanwhile reducing the entanglement between spin pairs next to the defect. It is of absolute relevance that the couplings of the spin chain with both the uniform and the local fields are described by terms which commute with the bare exchange XX Hamiltonian. This means that a time variation of the control parameters $h$ and $\alpha$ induces a fully adiabatic dynamics as non-equilibrium configurations are never accessed.

When temperature $T$ is switched on, thermodynamic averages are given by Eqs. (3) weighted by fermionic population factors. As seen in Fig. 4 the spatial distribution of the magnetization is quite robust against temperature, essentially because of the energy gap between the localized level and the bottom of the band. This is also understood by noticing that the magnetic moment at the impurity, $\langle \sigma_{z}^{0} \rangle$, keeps finite at finite temperature. In fact, neglecting the contribution of the band amplitudes, we
find \( \langle \sigma_i^z \rangle \simeq -\frac{\alpha}{\sqrt{1+\alpha^2}} \tanh \frac{\alpha}{2} \), where the functional dependence of the hyperbolic tangent on \( T \) accounts for the temperature robustness.

As for the concurrences, a marked dependence on \( r \) survives at \( T \neq 0 \) and thermal entanglement is found for selected spin pairs, with \( C_{r,r+1} \) displaying a maximum at finite temperature for even \( r \), while it decreases monotonically for \( r \) odd. Although several systems which develop thermal entanglement are known, our model provides the additional possibility to select the spin pair for the enhancement (reduction) of entanglement.

Possible experimental studies of the above issues set in several frameworks. First of all, quasi-one dimensional magnetic compounds properly doped so as to introduce diluted magnetic impurities, might be considered \( \text{[26]} \) (to this respect, we verified that our results still hold in the case of two impurities, provided they are far enough from each other). In this case NMR imaging of the local magnetization near impurities could be performed, in analogy with the case of non-magnetic impurity \( \text{[19]} \); the same technique could be used to probe the spatially modulated susceptibility \( \text{[20]} \). Moreover, muon-spin relaxation experiments have been extensively performed to investigate the effects of magnetic doping in high-\( T_c \) cuprates \( \text{[28]} \) and might also be proper tools for testing our findings, since the muon acts as both the impurity and the probe for the local magnetic arrangement \( \text{[20]} \). In this framework, however, no external tuning of the parameter \( \alpha \) is possible, as its value would result from the magnetic moment of the impurity, uniquely fixed by the dopant properties. Nonetheless, control upon the uniform field would still be feasible. Another possible implementation is suggested by the recent proposal \( \text{[30]} \) for realizing effective spin systems by coupled micro-cavities: in this case, the uniform magnetic field might be tuned by varying the frequencies of the driving lasers, while the impurity term could result from the level structure of the micro-cavity representing the spin sitting at the site of the impurity. Atomic condensates in optical lattices can also be considered, as it has been shown that they can simulate bosonic and fermionic models which can be mapped to the XX model in a transverse field in its quasi-long-range ordered phase \( \text{[31]} \).

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