Entanglement in quantum computers described by the *XXZ* model with defects

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We investigate on how to generate maximally entangled states in systems characterized by the Hamiltonian of the *XXZ* model with defects. Some proposed quantum computers are described by such a model. Defects embedded in this otherwise homogeneous spin chain are used to obtain Einstein-Podolsky-Rosen and *W* states. It is well known that a large defect localizes an excitation on the defect site. We can then consider a few identical and large defects to create a subsystem whose eigenstates are entangled. Here, we examine the cases of one and two excitations.

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I. INTRODUCTION

Since qubits are two-level systems, they are naturally modeled by spin-1/2 particles. Understanding spin chains is therefore very useful in the study of quantum computers (QCs). Interaction between qubits corresponds then to interaction between spins. One of the major problems of condensed-matter-based quantum computers is that the interaction between qubits cannot be turned on and off when desired, and the quantum computer eigenstates soon become a linear superposition of a large number of noninteracting multiqubit states [1]. However, when performing computations, we would like to operate with well-defined states, in other words, we would like to entangle just some specific states. In order to do so, we refer to two important characteristic of most proposed QCs, which are the following: the energy difference between the qubits states is large compared to the qubit-qubit interaction and it can be individually controlled [2,3]. In the QC based on electrons on helium, for example, the level spacing of each qubit is controlled by electrodes placed beneath the helium surface [3]. The possibility of individually controlled qubit energies allows us to entangle just some selected qubits by tuning them in resonance.

A fundamental requirement for the realization of quantum computation, quantum teleportation, and some protocols of quantum cryptography is the generation of highly entangled quantum states. The maximally bipartite pure-state entanglement is identified with the Bell or the Einstein-Podolsky-Rosen (EPR) state $(1/\sqrt{2})(|10\rangle+|01\rangle)$ [4]. Dür *et al* showed that there are two different kinds of genuine tripartite pure-state entanglement: the maximally entangled Greenberger-Horne-Zeilinger (GHZ) state [5] and the so called *W* state [6]. The *W* state is the state of three qubits that retains a maximal amount of bipartite entanglement when any one of the three qubits is traced out. It is written as $(1/\sqrt{3})(|100\rangle+|010\rangle+|001\rangle)$.

There is a large list of references dedicated to the problem of entanglement. There have been attempts to characterize qualitatively and quantitatively the entanglement properties of multiparticle systems [7]. Several proposals of how to prepare entangled states in different kinds of systems have also been presented [8]. Some papers investigated the entanglement between spins in a one-dimensional Heisenberg chain [9,10], which is similar to what we intend to do here. Contrary to the last cited papers, we consider a chain with defects and study their role in entangling states. In a system where all qubits are in resonance but one, a defect corresponds to the qubit whose level spacing is different from the others.

In this paper, we investigate on how to entangle selected qubits in a system described by a strongly anisotropic one-dimensional *XXZ* model with defects. This is the model used to describe the quantum computer based on electrons on helium [3]. Since the coupling falls down quickly with the interqubit distance, we consider only the nearest-neighbor interaction. The ground state of the system corresponds to all spins pointing down and excitations correspond to spins pointing up. The interaction can only move excitations one site to the left or to the right, so the number of excitations is constant. We analyze systems with one or two spins up. In the case of one single excitation, we show how the defects of the chain can be used to maximally entangle two qubits. In the case of two excitations, we show how EPR states and *W* states can be obtained.

II. GENERATION OF MAXIMALLY ENTANGLED STATES OF SELECTED QUBITS

The Hamiltonian of the *XXZ* model with defects is

$$H=\sum_{n=1}^{N}\frac{\varepsilon_n}{2}\sigma_n^z+\frac{B}{2}\sum_{n=1}^{N-1}\left[\frac{\Delta}{2}\sigma_n^z\sigma_{n+1}^z+\frac{1}{2}H_{\mathrm{hop}}\right],$$

$$H_{\mathrm{hop}}=(\sigma_n^+\sigma_{n+1}^-+\sigma_n^-\sigma_{n+1}^+), \tag{1}$$

where $\hbar=1$, $\sigma^{z,+,-}$ are Pauli matrices, and ε_n gives the energy difference between the two states of qubit *n*. There are *N* qubits. Here, we consider a spin chain with free boundaries, which explains why the second sum runs over $n=1,\ldots,N-1$. In strongly anisotropic systems (such as the QC based on electrons on helium), the parameter Δ is much larger than *B*. The last term in the Hamiltonian, H_{hop}, is responsible for the propagation of the excitation.

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The ground state corresponds to all spins pointing down and its energy is $\mathcal{E}_0=-\Sigma_{n=1}^{N}\varepsilon_n/2+(N-1)B\Delta/4$, which we will set equal to zero. Moreover, to simplify our analysis we consider only positive values for the parameters of the Hamiltonian.

To address the different states of the system, we use a notation that is common in the study of spin chains with the Bethe ansatz [11,12]. The state corresponding to one single excitation on site n, that is $|\downarrow_1\downarrow_2\cdots\downarrow_{n-1}\uparrow_n\downarrow_{n+1}\cdots\downarrow_N\rangle$, is simply written as $\phi(n)$. The state of two excitations, one on site n and the other one on site m, is $\phi(n,m)$, which is a simplified notation for $|\downarrow_1\cdots\uparrow_n\cdots\uparrow_m\cdots\downarrow_N\rangle$.

A. One excitation

Let us first examine the case of just one excitation. Assume that there are only two defects, whose level spacings are ε_0+g, while the level spacing of all other qubits is ε_0. By choosing g much larger than the interaction strength B, we generate maximally entangled states corresponding to linear combinations of the two defects.

The energy of states, which have the excitation on any site except on the defects, lies within the band $\mathcal{E}_1\pm B$, where $\mathcal{E}_1=\varepsilon_0-B\Delta$ [11,12]. If g is much larger than B, an excitation on one of the defects will have energy out of the band. Therefore, the two resonant defects can be treated separately from all other states by the perturbation theory. It is as if we were working with only two sites. An excitation initially created on one defect will only oscillate between the two defects. All intermediate states for the excitation to go from one defect to the other are virtual states. The frequency of these oscillations depend on the distance between the two different qubits. Their separation determines in which order of the perturbation theory they are connected.

The two states corresponding to superpositions of an excitation on a defect on site n_0 and an excitation on a defect on site m_0 are the following EPR states:

$$\psi_{\pm}=\frac{1}{\sqrt{2}}[\phi(n_0)\pm\phi(m_0)], \tag{2}$$

where $\phi(n_0)=|\uparrow_{n_0}\downarrow_{m_0}\rangle$ and $\phi(m_0)=|\downarrow_{n_0}\uparrow_{m_0}\rangle$.

If the two defects are next to each other ($m_0=n_0+1$), the energies of these two entangled states in the first order are

$$E_{\pm}=\mathcal{E}_1+g\pm B/2. \tag{3}$$

We just need to diagonalize a two-dimensional submatrix, whose diagonal elements are $\mathcal{E}_1+g$ and off-diagonal elements are $B/2$. After shifting the energy levels by a second-order correction $B^2/4(g+B/2)$, they agree very well with a complete numerical diagonalization of a long chain with g much larger than B.

If the second defect is located on site n_0+2 we have to go straight to the second order and diagonalize a matrix whose diagonal elements are $\mathcal{E}_1+g+B^2/(2g)$ and off-diagonal elements are $B^2/(4g)$. The two energies become much closer,

$$\begin{aligned} E_{+}&=\mathcal{E}_1+g+3B^2/(4g),\\ E_{-}&=\mathcal{E}_1+g+B^2/(4g). \end{aligned} \tag{4}$$

The more distant the two defects are, the closer the energies of the two entangled states will be, since we have to go to higher orders to find them.

Suppose that an initial state is prepared, which has an excitation on the defect n_0. Let us now see how long we have to wait for it to become a maximally entangled state such as given by Eq. (2). This excitation oscillates between the defect n_0 and the defect m_0. The probability to find it later in time on site n_0 is

$$P_{\phi(n_0)}(t)=\frac{1+\cos[(E_{+}-E_{-})t]}{2}, \tag{5}$$

while the probability to find it on m_0 is

$$P_{\phi(m_0)}(t)=\frac{1-\cos[(E_{+}-E_{-})t]}{2}. \tag{6}$$

It is seen from Eqs. (5) and (6) that the period of oscillation of the excitation between the defects is inversely proportional to the energy difference of the states ψ_{+} and ψ_{-}. Such a period depends on the number μ of sites between the defects as $T_{\mu}=T_0(2g/B)^{\mu}$, where $T_0=2\pi/B$. The maximally entangled states (2) are obtained when $P_{\phi(n_0)}=P_{\phi(m_0)}=1/2$. The further the defects are from each other, the longer we will have to wait for an EPR type of state to be created. It is clear, however, that by tuning two qubits in resonance with energies very different from all the others, we can entangle even remote qubits.

At the moment where a maximally entangled state is created, in order for it to be kept this way, the two defects have to be detuned. The difference in energy between these two excited qubits should become much larger than the interaction strength between them (of course, the defects and the other qubits are still completely out of resonance). How fast this detuning should be done depends on how much close we want to keep our state from a perfect EPR state.

Similarly, a W state can be built with three resonant defects, but we postpone the description of how to create such states to the following section where we have the more interesting case of two excitations.

B. Two excitations

In order to create EPR states and W states with two excitations we make use of the anisotropy of the system. Because Δ is much larger than B, two excitations next to each other have energy much larger than any state where they are separated. The energy of any two free excitations lies inside the band $2\mathcal{E}_1\pm 2B$, while the bound pair states have energy within a much narrower band $2\mathcal{E}_1+B\Delta+B/2\Delta\pm B/2\Delta$ [11,12]. As a consequence, the bound pair states can be treated separately from all other two-excitation states [12]. They are connected in the second order of the perturbation

theory, which explains the narrow bandwidth $B^2/(B\Delta) \equiv B/\Delta$. Any intermediate and dissociated state is a virtual state.

Suppose that there is only one defect on site n_0 with level spacing ε_0+g. If g is much larger than $B/2\Delta$, the bound pairs with one excitation on the defect have energy out of the narrow band. They form the EPR states

$$\psi_{\pm}=\frac{1}{\sqrt{2}}[\phi(n_0-1,n_0)\pm\phi(n_0,n_0+1)], \tag{7}$$

where $\phi(n_0-1,n_0)=|\uparrow_{n_0-1}\uparrow_{n_0}\downarrow_{n_0+1}\rangle$ and $\phi(n_0,n_0+1)=|\downarrow_{n_0-1}\uparrow_{n_0}\uparrow_{n_0+1}\rangle$. Their energies are

$$E_{\pm}=2\mathcal{E}_1+g+B\Delta+\frac{B}{4\Delta}+\frac{B^2}{4(B\Delta+g)}\pm\frac{B^2}{4(B\Delta+g)}. \tag{8}$$

By preparing an initial state with one excitation on site n_0-1 and the other on the defect site n_0, following Eqs. (5) and (6), we will obtain an EPR state at every instant of time

$$t_k=2(B\Delta+g)[\pi/2+k\pi]/B^2, \tag{9}$$

where k is an integer number.

Using the anisotropy, several other types of EPR states can be created. With three defects on sites n_0, n_0+1, and n_0+2, if they all have the same level spacing ε_0+g and $g \gg B/(2\Delta)$, we would have linear combinations of the bound pairs $\phi(n_0,n_0+1)=|\uparrow_{n_0}\uparrow_{n_0+1}\downarrow_{n_0+2}\rangle$ and $\phi(n_0+1,n_0+2)=|\downarrow_{n_0}\uparrow_{n_0+1}\uparrow_{n_0+2}\rangle$. As mentioned above, these states are connected in the second order of the perturbation theory.

Another EPR state that can be created with these three defects involves the states $\phi(n_0,n_0+1)=|\uparrow_{n_0}\uparrow_{n_0+1}\downarrow_{n_0+2}\rangle$ and $\phi(n_0,n_0+2)=|\uparrow_{n_0}\downarrow_{n_0+1}\uparrow_{n_0+2}\rangle$. The level spacing of the defect on site n_0+2 is now $\varepsilon_0+g+B\Delta$. The difference $B\Delta$ from the other two defects allows the entanglement between the bound pair $\phi(n_0,n_0+1)$ and the state $\phi(n_0,n_0+2)$. These states are connected in the first order in B. The advantage of this entanglement is that the period of oscillations between an initial state $\phi(n_0,n_0+1)$ and the state $\phi(n_0,n_0+2)$ is much shorter than oscillations between bound pairs. On the other hand, to guarantee that $\phi(n_0,n_0+1)$ and $\phi(n_0,n_0+2)$ are the only two states of the entanglement, g has to be larger than B, instead of just larger than $B/(2\Delta)$ as in the bound pair case.

This anisotropic chain with defects can also be used to create a W state. In order to do so we choose four equal defects on sites n_0, n_0+1, n_0+2, and n_0+3 with level spacings ε_0+g and g much larger than $B/(2\Delta)$. The bound pairs on the defects are much higher in energy than any other state and they can be treated separately. It becomes a good approximation to say that three of the eigenfunctions of the total Hamiltonian (1) will correspond to linear combinations of the bound pairs $\phi(n_0,n_0+1)=|\uparrow_{n_0}\uparrow_{n_0+1}\downarrow_{n_0+2}\downarrow_{n_0+3}\rangle$, $\phi(n_0+1,n_0+2)=|\downarrow_{n_0}\uparrow_{n_0+1}\uparrow_{n_0+2}\downarrow_{n_0+3}\rangle$, and $\phi(n_0+2,n_0+3)=|\downarrow_{n_0}\downarrow_{n_0+1}\uparrow_{n_0+2}\uparrow_{n_0+3}\rangle$. Such eigenfunctions and their correspondent eigenvalues are obtained from the diagonalization of the following tridiagonal submatrix:

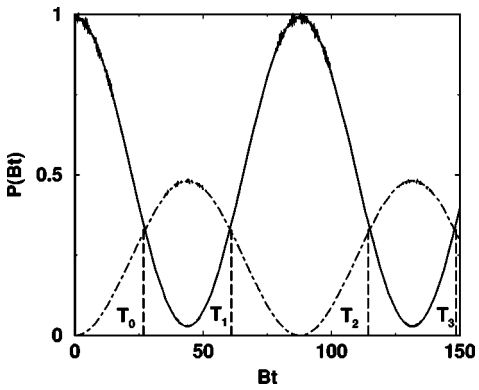

FIG. 1. We considered a chain with 12 qubits, $B=1$, and $\Delta=10$. The defects are located on sites n_0, n_0+1, n_0+2, and n_0+3, where $n_0=3$ and $g=B\Delta$. The solid line gives the probability in time to find the initial state $\phi(n_0+1,n_0+2)$. Both probabilities to find state $\phi(n_0,n_0+1)$ and state $\phi(n_0+2,n_0+3)$ coincide and they are given by the dot-dashed line. The vertical dashed lines correspond to the instants of time, $T_k=Bt_k$, where we have a W state.

$$\begin{pmatrix} E^{(0)}+r+s & r & 0 \\ r & E^{(0)}+2r & r \\ 0 & r & E^{(0)}+r+s \end{pmatrix}.$$

Above $r=B/(4\Delta)$, $s=B^2/[4(B\Delta+g)]$ and $E^{(0)}=2\mathcal{E}_1+B\Delta+2g$. The difference in energy between the diagonal element in the middle of the matrix and the diagonal elements at the edges, $B/(4\Delta)-B^2/[4\Delta(B\Delta+g)]$, exists because states $\phi(n_0,n_0+1)$ and $\phi(n_0+2,n_0+3)$ make virtual transitions to states that are out of the ''subchain'' created by the defects.

The eigenvalues are therefore

$$E_1=E^{(0)}+\frac{4B^2\Delta+3Bg-Bu}{8\Delta(B\Delta+g)},$$

$$E_2=E^{(0)}+\frac{B(2B\Delta+g)}{4\Delta(B\Delta+g)},$$

$$E_3=E^{(0)}+\frac{4B^2\Delta+3Bg+Bu}{8\Delta(B\Delta+g)},$$

where $u=\sqrt{8B^2\Delta^2+16B\Delta g+9g^2}$.

To generate a W state we have to prepare an initial state with excitations on n_0+1 and n_0+2, since this state is the only one among the three states, which is connected to the two others in the second order. The probability in time to obtain the initial state $\phi(n_0+1,n_0+2)$ is

$$P_{\phi(n_0+1,n_0+2)}(t)=\frac{1+\cos[(E_3-E_1)t]}{2}. \tag{10}$$

The probability to find state $\phi(n_0,n_0+1)$ or state $\phi(n_0+2,n_0+3)$ is the same and is given by

$$P_{\phi(n_0,n_0+1)}(t)=\frac{1-\cos[(E_3-E_1)t]}{4}. \quad (11)$$

The W state appears at the following instants of time (see Fig. 1):

$$t_k=\frac{(-1)^k\arccos(-1/3)+2\pi[k-\mathrm{int}(k/2)]}{E_3-E_1}, \quad (12)$$

where k is an integer and int$(k/2)$ correponds to the integer part of the ratio $k/2$.

As pointed out in the preceding section, for the maximally entangled state to be kept this way, at the moment where it is generated, the level spacings of the qubits involved in the process should become different. This detuning should be larger than the interaction strength among them.

The W state with the bound pairs $\phi(n_0,n_0+1)$, $\phi(n_0+1,n_0+2)$, and $\phi(n_0+2,n_0+3)$ can also be created with only two defects located on sites n_0-1 and n_0+4, but here the situation is more delicate. As before, g has to be larger than the bandwidth of the bound pair band, but it cannot be close to $B\Delta$, because this would create resonances with states that have one excitation on the defect [12].

III. CONCLUSION

We have investigated on how the defects of a spin chain with strongly anisotropic coupling can be used to obtain EPR and W states. These are the states used in the study of bipartite and tripartite entanglement, respectively. We considered the XXZ model with defects, for this is the model used to describe some quantum computers, such as the one based on electrons on helium [3]. It was shown that even though the interaction among qubits is on all the time, we can determine among which qubits the interaction is actually effective by controlling the level spacings. This allows the entangling of only certain chosen sites.

Over the years, magnetochemists have refined the art of designing and growing crystals of quasi-one-dimensional magnetic materials. These systems should therefore be useful in the study of entanglement.

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