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LETTER TO THE EDITOR

Antiresonance and interaction-induced localization in spin and qubit chains with defects

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Abstract

We study a spin chain with an anisotropic XXZ coupling in a magnetic field. Such a chain models several proposed types of quantum computers. The chain contains a defect with a different on-site energy. The interaction between excitations leads to the onset of two-excitation states localized next to the defect. In a resonant situation scattering of excitations on each other might cause decay of an excitation localized on the defect. We find that destructive many-particle quantum interference *eliminates* this decay. Numerical results confirm the analytical predictions.

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An important motivation for making a quantum computer as envisaged by Feynman is to simulate real quantum systems. Disordered systems with interacting excitations are of particular interest in this context. An important class of such systems are disordered spin-1/2 systems. The spin–spin interaction leads to a complicated excitation spectrum, that has been described only in special cases where the system is integrable [1, 2].

A spin-1/2 system can be modelled by a set of interacting two-level subsystems, qubits. Controlled qubits, with interqubit coupling that is not turned on and off, are basic elements of several proposed implementations of a quantum computer (QC) [3–8]. Qubit energies can be often individually varied. This allows one to explore resonant situations in a multiply excited system. In contrast to naturally occurring many-particle resonances in condensed-matter systems, in a QC the parameters can be tuned into resonance in a controlled way.

In this letter we show that a simple spin chain with a defect displays new types of localized two-excitation states and destructive two-excitation interference, i.e., an effect of two-excitation antiresonance. This is a result of the interplay between disorder and interaction. In turn, localization of excitations on individual qubits is important for quantum computing, because the qubits can be then prepared in desired states, which are not destroyed by other excitations.

We consider a spin chain in a magnetic field. The defect corresponds to ‘diagonal disorder’: the spin energy on the defect site differs from that on the host site (for example, the magnetic field on the defect site differs from the field on the host sites). The exchange coupling is anisotropic and is described by the XXZ model, which applies to several proposed quantum computers. The Hamiltonian of the chain with a defect on site n_0 is of the form

$$H = \frac{1}{2} \sum_n \varepsilon^{(n)} \sigma_n^z + \frac{1}{4} \sum_n \sum_{i=x,y,z} J_{ii} \sigma_n^i \sigma_{n+1}^i$$

$$\varepsilon^{(n)} = \varepsilon + g \delta_{n,n_0} \quad J_{xx} = J_{yy} = J \quad J_{zz} = J \Delta. \quad (1)$$

Here, σ_n^i are the Pauli matrices and $\varepsilon^{(n)}$ is the spin-flip energy on site n . All $\varepsilon^{(n)}$ are the same except for the site $n = n_0$. This is not the condition in which a QC should normally operate, because excitations are mostly delocalized and are scattered by each other. But even here, as we show, a multiply excited system has strongly localized states.

In equation (1), the defect is characterized by the excess energy g . The parameter Δ determines the coupling anisotropy. We assume that $|\Delta| \gg 1$, as in the case of a QC based on electrons on helium, for example [5]. To simplify notation, we further assume that the spin coupling is antiferromagnetic: $J, \Delta > 0$.

For large on-site energies $\varepsilon^{(n)}$, the ground state of the system corresponds to all spins pointing downwards, $\langle \sigma_n^z \rangle = -1$. The number of excitations is the number of spins pointing upwards. It is conserved, because the total spin projection $\sum \sigma_n^z$ commutes with H . In what follows we count energy off from the ground-state energy.

Single-spin excitations for the Hamiltonian (1) are well understood [9]. In an infinite chain they are either of the spin-wave type (‘magnons’) or localized on the defect. The magnon energies form a band of width $2J$ centred at $\varepsilon_1 = \varepsilon - J\Delta$. The localized excitation has energy $\varepsilon_1 + (g^2 + J^2)^{1/2} \text{sgn}g$. We will be interested in the case $g \gg J$, when the excitation is strongly localized on the defect.

Two-spin excitations are well understood for an ideal chain [10]. For strong anisotropy, $\Delta \gg 1$, they are either uncoupled magnons or bound pairs (BPs) of flipped neighbouring spins that propagate together. The two-magnon energy band is centred at $2\varepsilon_1$ and has a width of $4J$. When excitations are on neighbouring sites, their energy is changed by $J\Delta \gg J$, because of the term $(J\Delta/4) \sum_n \sigma_n^z \sigma_{n+1}^z$ in H (1). Respectively, the BP band is centred at $E_{\text{BP}}^{(0)} \approx 2\varepsilon_1 + J\Delta$ and is well separated from the two-magnon band. Motion of a BP occurs via virtual dissociation, where one excitation hops to a neighbouring nonexcited site and then the second excitation moves next to it. The bandwidth resulting from this process can be calculated by perturbation theory in $1/\Delta$. It is given by J/Δ and is parametrically smaller than the magnon bandwidth.

In the presence of a defect, there emerges an additional two-excitation state where one excitation is localized on the defect and the other is in an extended (magnon-type) state. We call it a localized–delocalized pair (LDP). The LDP band is centred at $E_{\text{LDP}}^{(0)} \approx 2\varepsilon_1 + g$ and has a width of the one-magnon band $2J$ (see below).

If the LDP energy band overlaps with the BP band, one would expect that the two types of excitations mix together. In other words, the propagating magnon of an LDP can scatter off the localized excitation, and they together would move away from the defect as a BP. This would lead to magnon-induced decay of a localized excitation. We show below that the decay does not happen because of destructive quantum interference.

The wavefunction of a chain with two excitations is a linear superposition $\psi_2 = \sum_{n < m} a(n, m) \phi(n, m)$, where $\phi(n, m)$ is the state where the spins on sites n and m are pointing upwards and all other spins are pointing downwards. From equation (1), the Schrödinger

equation for the coefficients $a(n, m)$ has the form

$$(2\varepsilon_1 + g\delta_{n,n_0} + g\delta_{m,n_0} + J\Delta\delta_{m,n+1})a(n, m) + (J/2) \sum_{k=\pm 1} [a(n+k, m) + a(n, m+k)] = E_2 a(n, m). \quad (2)$$

Here, E_2 is the energy of a two-excitation state counted off from the ground-state energy, and $a(n, n) \equiv 0$ (two excitations may not be placed on one site).

The defect may lead to a localized state of a bound pair with energy close to the energy of a propagating pair $E_{\text{BP}}^{(0)}$. This state is centred on sites $(n_0 + 1, n_0 + 2)$, or equivalently $(n_0 - 1, n_0 - 2)$. To show this we seek the major term in the solution of equation (2) in the form

$$a^{(0)}(n, m) = A\delta_{n,n_0+1}\delta_{m,n_0+2} + C_1 e^{i\theta_1(n-n_0-2)}\delta_{m,n+1}\Theta(n-n_0-2) + (C_2 e^{i\theta_2(m-n_0-2)} + C_2' e^{-i\theta_2(m-n_0-2)})\delta_{n,n_0}\Theta(m-n_0-2). \quad (3)$$

Here, A is the amplitude of the pair on sites $(n_0 + 1, n_0 + 2)$, C_1 is the amplitude of a BP propagating away from the defect with wave number θ_1 , and C_2 and C_2' are the amplitudes of LDP waves in which one excitation is on the defect whereas the other is propagating away from and towards the defect, respectively, with wave number θ_2 ; $\Theta(m)$ is the step function, which is equal to 1 for $m \geq 0$ and 0 for $m < 0$. For concreteness, we consider excitations 'to the right' from the defect, $m > n_0$. They do not mix with the excitations 'to the left', to first order in Δ^{-1} .

The BP localized next to the defect would be described by the wavefunction (3) with $C_2' = 0$ and with $\text{Im } \theta_{1,2} > 0$. On the other hand, resonant mixing of LDPs and BPs would be described as scattering of an LDP wave incident on the defect ($C_2' = 1, \theta_2 > 0$) into a reflected LDP with amplitude C_2 and a BP with amplitude C_1 and $\theta_1 > 0$.

Equations (2) and (3) with $n = m - 1 > n_0 + 2$ and $n = n_0, m > n_0 + 3$ give, respectively, the dispersion laws of BPs and LDPs far from the defect. From equation (2), a BP on sites $(n, n + 1)$ is directly coupled to nonresonant dissociated pairs on sites $(n - 1, n + 1)$ and $(n, n + 2)$. Similarly, an LDP on sites (n_0, m) is coupled to resonant pairs on sites $(n_0, m \pm 1)$ and to nonresonant pairs on sites $(n_0 \pm 1, m)$. Finding the amplitudes of the nonresonant pairs to first order in Δ^{-1} from equation (2) and substituting them back into the equations for C_1 and C_2 , we obtain, respectively, the BP and LDP dispersion laws:

$$\begin{aligned} E_{\text{BP}}(\theta) &= E_{\text{BP}}^{(0)} + (J/2\Delta) \cos \theta & E_{\text{BP}}^{(0)} &= 2\varepsilon_1 + J\Delta + (J/2\Delta) \\ E_{\text{LDP}}(\theta) &= E_{\text{LDP}}^{(0)} + J \cos \theta & E_{\text{LDP}}^{(0)} &= 2\varepsilon_1 + g + (J/2\Delta) \end{aligned} \quad (4)$$

(the renormalization of the energy spectrum is calculated for $|E_2 - E_{\text{BP}}^{(0)}| \lesssim J$).

Wave mixing near the defect can be described in a similar way by writing equations (2) and (3) for the sites $(n_0 + 2, n_0 + 3)$, $(n_0 + 1, n_0 + 2)$ and $(n_0, n_0 + 2)$ and eliminating nonresonant pair states by perturbation theory. For energies E_2 close to $E_{\text{BP}}^{(0)}$ this gives

$$C_1 e^{-i\theta_1} = A + C_2 e^{i\theta_2} + C_2' e^{-i\theta_2} \quad A = C_2 e^{-i\theta_2} + C_2' e^{i\theta_2} + \Delta^{-1}(C_2 + C_2') \quad (5)$$

$$[4(J\Delta - g - J \cos \theta_2) - J\Delta^{-1}]A + 2J(C_2 + C_2') + J\Delta^{-1}(C_2 e^{i\theta_2} + C_2' e^{-i\theta_2}) + J\Delta^{-1}C_1 = 0 \quad (6)$$

(the corrections $\sim \Delta^{-1}$ to the first equation (5) come from higher order terms of the perturbation theory; they are not important for the present calculation).

Equations (5) and (6) contain two dimensionless parameters, Δ and $\alpha = (J\Delta - g)/J$, which are related to the three energy scales in the system: the distance between the BP and LDP bands $J\Delta - g$ and the LDP and BP bandwidths J and J/Δ .

To find the state localized on sites $(n_0 + 1, n_0 + 2)$, we set $C'_2 = 0$. Then, for $\Delta \gg 1$ the solution of equations (5) and (6) can be approximated by $\exp(-i\theta_2) \approx 2J^{-1}(J\Delta - g) + (2\Delta)^{-1}[\exp(i\theta_1) - 1]$ (the term $\propto \Delta^{-1}$ is important only for $|\alpha| \gg 1$ and should be modified for $|\alpha| \sim 1$). The energy of the localized state E_{loc} and the reciprocal localization lengths $\text{Im } \theta_{1,2}$ are obtained by substituting this expression into the equation $E_{\text{loc}} = E_{\text{BP}}(\theta_1) = E_{\text{LDP}}(\theta_2)$.

For $|\alpha| \gg 1$ the BP and LDP bands are far from each other, and

$$E_{\text{loc}} - E_{\text{BP}}^{(0)} \approx \frac{J}{4\Delta} \frac{\Delta^2 - 2\alpha\Delta + 2\alpha^2}{\alpha(\Delta - \alpha)} \quad \alpha = \frac{J\Delta - g}{J}. \quad (7)$$

The localized state amplitude is $A \sim 1$. The state is mostly hybridized with the BP band, with $C_1/A \approx \alpha/(\Delta - \alpha)$ and $\text{Im } \theta_1 = \ln[(\Delta - \alpha)/\alpha]$. The admixture of the LDP band is small, $C_2/A \sim 1/2\alpha \ll 1$. In a way, the localized state is a 'surface' state of the BP band, with the role of the surface being played by the defect. It emerges for $\alpha < \Delta/2$.

As the BP and LDP bands approach each other and α decreases, the energy E_{loc} moves away from the BP band. The localized state becomes stronger hybridized with the LDP band than with the BP band, with $C_2/A \approx 1/2\alpha$ and $C_1/A \sim \alpha/\Delta \ll 1$ for $|\alpha| \ll \Delta$. The energy separation from the LDP band is

$$E_{\text{loc}} - E_{\text{LDP}}^{(0)} \approx J[\alpha + (4\alpha)^{-1}] \quad (\alpha \sim 1). \quad (8)$$

It is of the order of the LDP bandwidth J . The localized state exists for $|\alpha| > 1/2$. The reciprocal localization length $\text{Im } \theta_2 = \ln(2|\alpha|)$ goes to zero as $|\alpha| \rightarrow 1/2$. As the BP band goes through the LDP band with varying $J\Delta - g$, the localized state first merges with the LDP band and disappears for $\alpha = 1/2$, and then is split off from the opposite side of the LDP band for $\alpha = -1/2$. The dependence of E_{loc} on parameters is discussed elsewhere [11] in more detail, along with the onset of other localized two-excitation states.

We now consider the possibility of resonant mixing of LDP and BP states where the bands overlap. As mentioned above, we can do it by studying scattering of an LDP magnon off the excitation on the defect, i.e., by setting $C'_2 = 1$ in equations (5) and (6).

The LDP band is much broader than the BP band. From equations (4), LDPs with energies within the BP band have wave numbers θ_2 such that $\cos \theta_2 \approx (J\Delta - g)/J$. For such LDPs, $C_2 \approx -C'_2 = -1$ from equation (6), i.e., they are fully reflected from the defect. The amplitude of the BP wave is $C_1 = 0$, to zeroth order in Δ^{-1} . This happens even though the BP on sites $(n_0 + 1, n_0 + 2)$ has a large amplitude $A \approx 2i \sin \theta_2$.

The vanishing of the BP wave is a result of destructive interference, or antiresonance, as seen from the first of equations (5). The BP wave is coupled to both the pair $(n_0 + 1, n_0 + 2)$ and the pair on sites $(n_0, n_0 + 3)$, which has an amplitude $C_2 \exp(i\theta_2) + C'_2 \exp(-i\theta_2)$. For resonant, values of θ_2 the complex amplitudes of these two pairs are equal and opposite in sign; they cancel each other. One can show in a similar way that if a BP wave is incident on a defect, it will be fully reflected and no LDP waves will be excited. The absence of mixing of BP and LDP states at resonance is illustrated in figure 1, which is obtained by direct diagonalization of equation (2).

In this letter the effect of antiresonance has been found for many-particle excitations. It leads to localization of an excitation on a defect in an XXZ spin or qubit chain even where the excitation would be expected to decay via multiparticle scattering. We also found new localized two-excitation states. Their energy and localization length depend on the interrelation between the interaction anisotropy Δ^{-1} and the relative excess energy of an excitation on the defect site g/J . The results indicate that quantum computers can be advantageous for studying new many-body effects in systems with disorder.

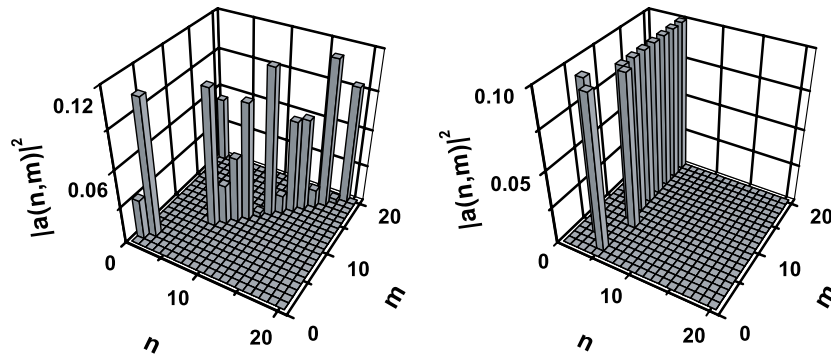


Figure 1. Amplitudes of two-excitation states on sites (n, m) in a periodic chain. Left and right panels show, respectively, bound pairs and localized–delocalized pairs with nearly same energy. The chain length is 20, the defect is on site $n_0 = 5$, and $g/J = \Delta = 10$. The BP is located on sites $m = n + 1$ and is well approximated by $a(n, n + 1) \propto \sin[10\pi(n - 6)/17]$. Because of the antiresonance, the BP amplitude is equal to zero on sites $n_0, n_0 \pm 1, n_0 \pm 2$. The LDP is located on sites (n_0, m) , with $m - n_0 > 1 \pmod{20}$, and is well described by $a(n_0, m) \propto \sin[(m - 1)\pi/2]$. The LDP is strongly hybridized with the pairs on sites $(n_0 + k, n_0 + 2k)$ ($k = \pm 1$), which have same amplitude, as expected.

From the standpoint of quantum computing, the many-particle localization that we discuss is important, because it is much easier to manipulate excitations when they are localized on individual qubits. Of interest for quantum computing is also the occurrence of different types of localized two-excitation states on neighbouring qubits. It allows creating on these qubits entangled Bell-type states, which are to some extent similar to recently studied entangled excitonic states in a quantum dot [12], but which appear in the present case in an extended system. We expect that coherent multi-qubit states can be created in a chain with a defect as well.

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