Even-Odd Effects of Heisenberg Chains on Long-range Interaction and Entanglement

Sangchul Oh, Mark Friesen, and Xuedong Hu

1Department of Physics, University at Buffalo, State University of New York, Buffalo, New York 14260-1500, USA
2Department of Physics, University of Wisconsin-Madison, Madison, Wisconsin 53706, USA

(Dated: July 26, 2010)

A strongly coupled Heisenberg chain provides an important channel for quantum communication through its many-body ground state. Yet, the nature of the effective interactions and the ability to mediate long-range entanglement differs significantly for chains of opposite parity. Here, we contrast the characters of even and odd-size chains when they are coupled to external qubits. Additional parity effects emerge in both cases, depending on the positions of the attached qubits. Some striking results include (i) the emergence of maximal entanglement and (ii) Ruderman-Kittel-Kasuya-Yosida (RKKY) interactions for qubits attached to an even chain, and (iii) the ability of chains of either parity to mediate qubit entanglement that is undiminished by distance.

PACS numbers: 03.67.Bg, 03.67.Lx, 75.10.Pq, 75.75.-c

The addition of even a single particle can have a striking effect on a quantum system. For example, spin-1/2 particles with antiferromagnetic exchange couplings tend to anti-align. The ground state of two coupled spins therefore has a compensated magnetic moment, with total spin \( S = 0 \). In contrast, a three-spin chain has an uncompensated moment, with total spin \( S = 1/2 \). Such even-odd parity effects have been observed recently in a number of geometries. For example, Hirjibehedin et al. \[1\] assembled antiferromagnetic Heisenberg chains of 1 to 10 manganese atoms on a copper nitride surface, revealing parity effects through scanning tunneling microscopy, while Micotti et al. \[2\] measured the local magnetic moments of CrCd and Cr8 rings using nuclear magnetic resonance methods.

Several attempts have been made to utilize strongly coupled spin chains as a medium for quantum communication, showing that long-distance entanglement can be generated in several types of spin chains \[3\], and that an odd-size Heisenberg chain can act as a spin bus for coupling remote qubits \[4\]. However, parity effects of the spin chain itself have not yet been clarified in these quantum information applications. In view of how dramatically parity can affect the ground state of a group of spins \[1\], it is important to investigate how parity effects compete with and emerge from the short-range exchange interaction in the spin-chain Hamiltonian, how the parity of a spin chain affects its capacity to mediate qubit interactions, and how these parity effects can be manipulated and taken advantage of.

In this Letter, we demonstrate dramatic even-odd parity effects of Heisenberg chains on induced long-range couplings and entanglement between remote qubits weakly attached to the chains. The effective interactions are obtained via perturbation calculations. At first order, an odd-size Heisenberg chain acts as a central spin to the qubits. The local magnetic moment of the chain at the qubit site determines the sign and strength of the effective coupling between them. In contrast, at second order, an even-size Heisenberg chain mediates an indirect RKKY interaction between any two external qubits \[5\]. The sign and strength of the interaction are determined by the spin-spin correlations within the chain. We show that these disparate coupling mechanisms allow the qubit couplings to be tuned from antiferromagnetic to ferromagnetic, and present intriguing opportunities for fabricating artificial spin lattices and superlattices.

\[\begin{align*}
\text{(a)} & & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & \text{N} \\
\text{(b)} & & \Delta & D_{1} & & D_{2} & & D_{3} & & & \\
\text{(c)} & & \Delta & D_{1}\prime & & D_{2}\prime & & & & & \\
\end{align*}\]

Figure 1: (color online). (a) Schematics of two qubits, \( A \) and \( B \), weakly attached to nodes \( i = 2 \) and \( j = 7 \) of a chain with \( N \) spins. The qubit perturbation affects the low energy manifolds of (b) an odd-size chain and (c) an even-size chain. (Left: unperturbed. Right: perturbed.) Here \( D_{1}, D_{2}, \) and \( Q \) denote low-lying doublet and quadruplet states, respectively. \( S \) denotes a singlet and \( T \) a triplet. \( \Delta \) is the ground energy gap of the chain. \( \delta \) is equal to \( |J_{A,i}| = |J_{B,j}| \) for an odd-size chain and \( |J_{A,B}(i,j)| \) for an even-size chain.

The model system we consider involves two qubits weakly coupled to a Heisenberg chain with \( N \) spin-1/2 particles, as shown in Fig. 1(a). Such a system can possibly be realized, for example, with quantum dot arrays, donor arrays, or magnetic molecules on a surface. The
total Hamiltonian for the two qubits and the chain is
\[ H = H_q + H_c + H_{qc}, \]
where \( H_q \) is the Zeeman term of the two qubits and taken to be zero for simplicity. The Hamiltonian of the spin chain with antiferromagnetic exchange couplings is
\[ H_c = \sum_{i=1}^{N} J_i s_i \cdot s_{i+1}, \]
where we take the uniform exchange couplings: \( J_i = J_0 \) for \( i = 1, \ldots, N - 1 \). For open chains, \( J_N = 0 \), while for rings, \( J_N = J_0 \) and \( s_{N+1} = s_1 \). A weak antiferromagnetic coupling between qubits, \( A \) and \( B \), and chain spins at nodes \( i \) and \( j \), respectively, is described by
\[ H_{qc} = J_{A,i} s_A \cdot s_i + J_{B,j} s_B \cdot s_j, \]
where \( 0 < J_{\alpha,i}/J_0 \ll 1 \), with \( \alpha = A, B \). In this work, we consider only two qubits attached to the chain. However, the general analysis is applicable to any number of qubits.

We first recall some basic properties of the spin-1/2 Heisenberg chain, defined in Eq. \( 2 \). (i) Partial solutions for \( H_c \) can be obtained via the Bethe ansatz \( \mathcal{B} \). (ii) The total spin operator \( s = \sum_{i=1}^{N} s_i \) and its \( z \) component \( s_z = \sum_{i=1}^{N} s_{iz} \) commute with \( H_c \), so their eigenvalues are good quantum numbers. (iii) Finite-size chains exhibit ground state energy gaps that vanish in the limit \( N \rightarrow \infty \). (iv) The nature of the ground-state manifold depends on the even-odd parity as well as the boundary conditions for the chain. We now derive the effective interactions when external qubits are coupled to such Heisenberg chains.

**Odd-size chains.** An odd-size Heisenberg chain with open boundary has a two-fold degenerate ground state, as depicted in Fig. \( 1 \)(b). The ground doublet \( \{ |0_c, 1_c \rangle, |1_c, 0_c \rangle \} \) has total spin \( s = \hbar/2 \) and \( s_z = \pm \hbar/2 \), similar to a single spin. The ground states of the odd-size chain can therefore be regarded as an extended object, whose spin-1/2 character is distributed over the entire chain, and is not localized at any given node. Thus, when the qubit coupling is weak, the odd-size chain can be effectively replaced by a single object called a “central spin”.

We derive the first-order effective Hamiltonian \( \mathcal{H} \) by projection: \( H_{\text{eff}} = (H_q + H_c) P + PH_{qc} P + \mathcal{O}(H_{qc}^2) \). The projection operator \( P = \sum_{i,m,n} \sigma_i c_{m,n} (|i\rangle \langle i|, m_A, n_B) \), with \( i, m, n = 0, 1 \), spans the qubit eigenstates and the ground state doublet of the chain. We thus obtain
\[ H_{\text{eff}} = J_{A,i} s_A \cdot S_c + J_{B,j} s_B \cdot S_c, \]
where the central spin operator \( S_c \) acting on the ground doublet is defined by \( S_{C,z} = s_z = \frac{1}{2} (|0_c\rangle \langle 0_c| - |1_c\rangle \langle 1_c|), S_{C,x} = \frac{1}{2} (|0_c\rangle \langle 1_c| + |1_c\rangle \langle 0_c|), \) and \( S_{C,y} = \frac{1}{2} (-i |0_c\rangle \langle 1_c| + i |1_c\rangle \langle 0_c|) \). The effective couplings \( J_{A,i}^* \) between the central spin and the qubits are given by
\[ J_{A,i}^* = \langle 0_c | \sigma_{iz} | 0_c \rangle = -\langle 1_c | \sigma_{iz} | 1_c \rangle = \langle 1_c | \sigma_{iz} | 0_c \rangle, \]
where Pauli matrices \( \sigma_i \) act on the \( i \)-th spin in the chain.

Equation \( 4 \) shows that qubits \( A \) and \( B \) may be coupled over long distance via the central spin \( C \). Furthermore, the effective coupling \( J_{A,i}^* \) of qubit \( \alpha \) to the central spin is given by the product of the bare coupling \( J_{A,i} \) and the local magnetic moment \( m_i/\mu_B = \langle 0_c | \sigma_{iz} | 0_c \rangle \) of the chain at the position where the qubit is attached. As shown in Fig. \( 2 \)(a), the local magnetic moments alternate, causing \( J_{A,i}^* \) to alternate as well. Thus, the antiferromagnetic (ferromagnetic) character of the effective central-spin-qubit interaction is determined by where the qubit is attached.

There are three possible combinations for the signs of \( J_{A,i}^* \) and \( J_{B,j}^* \), as determined by the parity of the attachment sites \( i \) and \( j \): (i) both positive (\( i \) and \( j \) both odd), (ii) one positive and one negative (\( i \) and \( j \) with opposite parity), and (iii) both negative (\( i \) and \( j \) both even). Let us rewrite Eq. \( 4 \) in the qubit-central spin-qubit (ACB) basis as
\[ H_{\text{eff}} = J_{A,i} (s_A \cdot s_C + \lambda s_B \cdot s_C), \]
where the magnitude of \( \lambda \equiv J_{B,j}^*/J_{A,i}^* \) can be tuned by the bare couplings \( J_{A,i} \) and \( J_{B,j} \) under the condition \( J_{A,i} \ll J_0 \). We now analyze each of these scenarios.

Case (i), where \( \lambda > 0 \). As depicted in Fig. \( 1 \)(b), the low-energy level ordering is given here by \( D_1 - D_2 - Q \). For the special case \( J_{A,i}^* = J_{B,j}^* > 0, \lambda = 1 \). The resulting ground-state doublet can be expressed as
\[ |G_1\rangle_{\text{ACB}} = \frac{1}{\sqrt{6}} (|001\rangle - 2|010\rangle + |100\rangle), \]
and its spin-flipped counterpart is \( |G_2\rangle_{\text{ACB}} \). More generally, the eigenstates will depend on \( \lambda \). We can quantify the entanglement in terms of the concurrence measure \( C \), obtaining \( C_{\text{ACB}} = 1/3 \) for either doublet state. Indeed, the concurrence between qubits \( A \) and \( B \), for any quantum superposition of \( |G_1\rangle \) and \( |G_2\rangle \), has the same value. We can further compute the concurrence in any spin pair, including the internal nodes of the chain, as shown in Fig. \( 2 \)(b). As noted in Ref. \( \mathcal{B} \), only nearest-neighbor spins in the chain exhibit a non-zero concurrence. On the other hand, the qubits and the central
spin have non-zero concurrence, except in the singular (but trivial) case of $\lambda = 0$, as shown in Fig. 3. The concurrence between $A$ and $B$ takes its peak value of $1/3$ when $\lambda = 1$, and vanishes when $\lambda \gg 1$, due to the competition between the qubits to form a singlet state with the central spin. The central spin is more entangled with the qubit having the larger antiferromagnetic coupling.

**Figure 3:** (color online). Concurrence between qubits $A$, $B$, and the central spin $C$ as a function of $\lambda$, as defined in Eq. (5).

Case (ii), where $\lambda < 0$. We take $J_{A,i}^* > 0$, $J_{B,j}^* < 0$. The low-energy states are now ordered $D_1' = Q - D_2'$, where two doublets $D_1'$ and $D_2'$ differ from $D_1$ and $D_2$. For $\lambda = -1$, for example, the ground state doublet $D_1'$ is $|G_1'\rangle_{ACB} = \frac{2 + \sqrt{3}}{3\sqrt{3}} |000\rangle - \frac{1}{\sqrt{3}} |101\rangle - \frac{1}{\sqrt{3}} |010\rangle$ and its spin-flipped counterpart is $|G_2'\rangle_{ACB}$. Fig. 3 shows that as $\lambda \to -\infty$, $C_{A,B}$ goes to $2/3$. The ground states becomes

$$|G_1'\rangle_{ACB} = \frac{1}{\sqrt{6}} (2|000\rangle - |010\rangle - |001\rangle).$$  

(7)

It is interesting to note that Eqs. (6) and (7) are identical if $A$ and $C$ are exchanged.

Case (iii), where $J_{A,i}^* < 0$ and $J_{B,j}^* < 0$, and the low energy states form a quadruplet. We find that the entanglement among spins $A$, $B$, and $C$ depends on the specific state, and is therefore not well defined.

**Even-size chains or rings.** The ground state of an even-size chain or ring is non-degenerate, as shown in Fig. 1(c). Its quantum numbers are $s = 0$ and $s_z = 0$, so that the first-order perturbation due to a weakly coupled qubit vanishes, and the second-order term is the leading order. In this case, the effective Hamiltonian for the ground state manifold is given by

$$H_{\text{eff}} = \mathcal{E}_0|0_c\rangle\langle 0_c| + J_{A,B}^* (i,j) \mathbf{S}_A \cdot \mathbf{S}_B,$$

(8)

with the induced effective coupling

$$J_{A,B}^* (i,j) = 2 \sum_{n_c \neq \mu} \frac{J_{A,i}^* J_{B,j}^*}{\mathcal{E}_0 - \mathcal{E}_n} |0_c|\langle \sigma_{\mu n_c}| n_c\rangle\langle n_c|\sigma_{\mu n_c}|0_c\rangle.$$

(9)

Here $|n_c\rangle$ and $\mathcal{E}_n$ are the excited eigenstates and eigenvalues of $H_c$. Note that the induced interaction is also isotropic and index $\mu$ in Eq. (9) is any of $x$, $y$, and $z$, but not the summation convention. Since the effective coupling involves virtually excited states of the chain, Eq. (9) can be expressed, alternatively, as $J_{A,B}^* (i,j) = 2J_{A,i}^* J_{B,j}^* \tilde{G}_{ij}(0)$, where $\tilde{G}_{ij}(\omega)$ is the Fourier transform of the time-dependent spin-spin correlation function for the ground state, $G_{ij}(t) = -i \langle 0_c|\sigma_{\mu i}(t)\sigma_{\mu j}|0_c\rangle$ with $\sigma_{\mu i}(t) = e^{iH_c t/\hbar}$ $\sigma_{\mu i} e^{-iH_c t/\hbar}$. While it is difficult to obtain a closed-form expression for $J_{A,B}^* (i,j)$, an approximate solution is given by

$$J_{A,B}^* (i,j) \approx -\frac{2J_{A,i}^* J_{B,j}^*}{\Delta} \langle 0_c|\sigma_{\mu i}\sigma_{\mu j}|0_c\rangle,$$

(10)

where $\Delta = \mathcal{E}_1 - \mathcal{E}_0$ is the ground energy gap of the chain and $\sum_{m\neq 0} \langle 0_c|\sigma_{\mu m\mu m}|0_c\rangle = \langle 0_c|\sigma_{\mu i}\sigma_{\mu j}|0_c\rangle$ may be used since $\langle 0_c|\sigma_{\mu i}|0_c\rangle = 0$.

We have computed $J_{A,B}^* (i,j)$, numerically, by two different methods. In the first method, we evaluate Eq. (9) using the unperturbed eigenvalues and eigenstates of the chain. In the second method, we diagonalize the full Hamiltonian (chain plus qubits), and compute the energy gap $\delta$ between the ground state and the lowest excited state, all within the manifold of the chain ground state. For odd qubit separations $|i-j|$ in Fig. 1(c), the ground state of the full system (chain plus qubits) is found to be a singlet, while the first excited state is found to be a triplet. The singlet-triplet energy gap $\delta$ is then given by $J_{A,B}^* (i,j) > 0$, just as if the two qubits experienced a direct, antiferromagnetic coupling.

**Figure 4:** (color online). Concurrence $C_{ij}$ of arbitrary spin pairs in the ground state of two even-size geometries ($N = 8$). (a) Qubits $A$ and $B$ are attached to sites 1 and 8 of an open chain. (b) $A$ and $B$ are attached to sites 1 and 4 of a ring.

After tracing out the chain degrees of freedom in the ground state of the full system, the reduced density matrix of qubits $A$ and $B$ is almost identical to a singlet $|\psi(-)\rangle_{AB} = \frac{1}{\sqrt{2}} (|01\rangle - |10\rangle)$. The two qubits are therefore maximally entangled, with concurrence $C_{A,B} \simeq 1$. The monogamous property of entanglement dictates that when qubits $A$ and $B$ are maximally entangled, they cannot also be entangled with the chain. Therefore, the ground state of the total system is approximately the product of the singlet state of the two qubits and the ground state of the chain, $|\Psi_0\rangle \approx |\psi(-)\rangle_{AB} \otimes |0_c\rangle$. Furthermore, the concurrence $C_{A,B}$ does not depend on the qubit coupling locations $i$ and $j$, provided the separation distance is odd. This is in contrast to the effective interaction, which decays slowly with qubit separation, as discussed below. In Fig. 4 we compute the concurrence
between spin pairs in two different geometries, for the case of odd qubit separation. We observe that pair-wise concurrence is translationally invariant for a ring geometry but not for an open chain.

For an even separation distance $|i-j|$ between the two qubits, the effective coupling is still determined by the ground state gap, $|J^*_{A,B}(i,j)| = \delta$. However, the coupling is now ferromagnetic, with $J^*_{A,B}(i,j) < 0$. The ground state of the full system is the product of a triplet state of qubits $A$ and $B$ and the ground state of the chain, $|\Psi_0\rangle = |T\rangle_{AB} \otimes |0\rangle_c$. The entanglement between the qubits depends on a specific superposition of the triplet.

Figure 5: (color online). (a) Spin-spin correlation $\langle \sigma_i \sigma_j \rangle$ for the ground state of the even-size chain with $N = 10$. (b) The RKKY interaction $J^*_{A,B}(1,1)$ normalized by $|J^*_{A,B}(1,1)|$. The labels “Exact” and “Approx.” correspond to Eqs. (9) and (10), respectively.

The alternating nature of $J^*_{A,B}(i,j)$ for even and odd qubit separations is indicative of RKKY effective interactions, as shown in Fig. 5. Note that for an open chain, $J^*_{A,B}(i,j)$ cannot be written as $J^*_{A,B}(|i-j|)$ because of the boundary effect. Eq. (10) suggests that the RKKY effective coupling $J^*_{A,B}(i,j)$ will exhibit a weak power-law decay, similar to the spin-spin correlations $|\Psi_0\rangle$. We can estimate the scaling of the RKKY interaction as follows. The ground state energy gap of the chain is bounded by $\Delta \sim \pi^2 J_0/2N$ [11]. Assuming a weak qubit-chain coupling $J_{A,i} = 10^{-2} \Delta$, we obtain a scaling estimate of $J^*_{A,B}(i,j) \sim 10^{-4} \pi^2 J_0/N$.

As demonstrated in this Letter, both ferromagnetic and antiferromagnetic couplings between qubits can arise in antiferromagnetically coupled chains. Such tunability provides opportunities to engineer new types of spin structures, as suggested in Fig. 6. As an example, we have sketched a spin superlattice with alternating ferromagnetic and antiferromagnetic effective interactions. The implications of such novel structures could range from new quantum correlations and phases to capabilities in the area of quantum information processing. We believe the system considered here can already be fabricated and tested with existing nanomagnet or trapped ion technologies [1, 2, 12, 13], while additional tunability could potentially be achieved in quantum dot systems.

In conclusion, we have shown that even-odd parity in a Heisenberg chain produces disparate interactions and entanglement properties between externally coupled qubits. An odd-size chain acts as a central spin to the qubits, with effective couplings that are determined by the local magnetic moment of the chain at the qubit site. On the other hand, an even-size chain mediates an RKKY interaction directly between the qubits. While an even-size chain produces a larger concurrence between the qubits, an odd-size chain provides stronger couplings and faster gate operations.

This work is supported by the DARPA/MTO QuEST program through a grant from AFOSR.

---

*Electronic address: sangchul@buffalo.edu

[1] C. F. Hirjibehedin, C. P. Lutz, and A. J. Heinrich, Science 312, 1021 (2006).
[2] E. Micotti, Y. Furukawa, K. Kumagai, S. Carretta, A. Lascialfari, F. Borsa, G. A. Timco, and R. E. P. Winpenny, Phys. Rev. Lett. 97, 267204 (2006).
[3] L. Campos Venuti, C. Degli Esposti Boschi, and M. Roncaglia, Phys. Rev. Lett. 96, 247206 (2006).
[4] M. Friesen, A. Biswas, X. Hu, and D. Lidar, Phys. Rev. Lett. 98, 230503 (2007).
[5] M.A. Ruderman and C. Kittel, Phys. Rev. 96, 99 (1954); T. Kasuya, Prog. Theor. Phys. 16, 45 (1956); K. Yoshida, Phys. Rev. 106, 893 (1957).
[6] H. Bethe, Z. Phys. 71, 205 (1931).
[7] C. Cohen-Tannoudji, J. Dupont-Roc, and G. Gryenberg, Atom-Photon Interactions (John Wiley & Sons Inc. New York, 1992).
[8] W. K. Wootters, Phys. Rev. Lett. 80, 2245 (1998).
[9] L. Amico, R. Fazio, A. Osterloh, and V. Vedral, Rev. Mod. Phys. 80, 517 (2008).
[10] A. Luther and I. Peschel, Phys. Rev. B 12, 3908 (1975).
[11] E. Lieb, T. Schultz, and D. Mattis, Ann. Phys. (N.Y.) 16, 407 (1961).
[12] L. Zhou, J. Wiebe, S. Lounis, E. Vedmedenko, F. Meier, S. Blügel, P.H. Dederichs, and R. Wiesendanger, Nature Physics (London) 6, 187 (2010).
[13] K. Kim, M.-S. Chang, S. Korenblit, R. Islam, E. E. Edwards, J. K. Freericks, G.-D. Lin, L.-M. Duan, C. Monroe, Nature (London) 465, 590 (2010).