Quantum phase transitions of spin chiral nanotubes

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Abstract

Recently many interesting magnetic nanostructures have been fabricated and much attention is arising on the rich magnetic properties that originate in the quantum effects eminent in the nanoscale world. One of the peculiar aspects of the quantum effects is the spin excitation gap. In the spin-1/2 low-dimensional systems, the spin gap often appears when the lattice dimerization or the frustration in the spin-spin interaction are introduced. In the present study, we investigate the ground-state property of the spin-1/2 antiferromagnetic spin chiral nanotubes with the spatial modulation in the spin-spin interaction. The ground-state phase diagrams of them are determined by observing the behavior of the expectation value of the Lieb-Schultz-Mattis slow-twist operator calculated by the quantum Monte Carlo method with the continuous-time loop algorithm. We discuss the relation between the characteristic of the topology of the phase diagram and the chiral vector of the nanotubes.

Key words: chiral nanotubes; spin gap; quantum Monte Carlo method

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1. Motivation

These days the experimental techniques have made a lot of progress and good experimentalists have synthesized the nanoscale magnets which realize the models that had been discussed only theoretically before. Among them are the BIP-TENO as the spin-1 two-leg ladder [1], the compound \([\text{CuCl}_2\text{tachH}_3\text{Cl}]\text{Cl}_2\) (tach=\textit{cis},\textit{trans}-1,3,5-triamino-cyclohexane) as the triangular spin nanotube [2], and the oxygen molecules adsorbed on the inner surface of the porous material as a many-leg spin tube [3]. The spin ladders [4] and tubes [5] have attracted attention in the course of the extensive studies on the low-dimensional magnets, part of which started from the discussions on the Haldane gap [6] of the one-dimensional spin chains. The appearance of the spin excitation gap is one of the interesting macroscopic quantum phenomena. In spin-1/2 systems, it occurs when the frustration in the spin-spin interaction or the lattice dimerization is introduced. A good example of the former case is the triangular spin nanotube [7] whose spontaneous dimerized and gapped ground state had been theoretically investigated [8] and now got a strong possibility of an experimental realization in the near future [2]. During the course of studies on the low-dimensional systems, the huge amount of studies on the carbon nanotubes...
were done in the 90’s, and the striking properties on the electric conductivity of the chiral nanotubes were found out. Namely, a carbon nanotube can be either a metal or a semiconductor, either of which is determined by the chiral vector [9,10,11].

With the great progress in experiments and theories, it is now interesting in both respects to ask, if the carbon atoms are replaced by some magnetic ions the chiral nanotubes and the antiferromagnetic superexchange interactions between them are introduced, are there any relations between the chiral vector and the magnetic properties analogous to the carbon nanotubes [12]?

The real experiments should be done in the near future. As for the numerical experiments, we take the spin-1/2 Heisenberg antiferromagnets on the chiral nanotubes made from the honeycomb strips as the simplest systems that the quantum effects bring about interesting properties. Remarkably, these models always enable us to perform numerical experiments by the quantum Monte Carlo method without suffering from the notorious negative sign problem [13]. This is not generally the case for the spin nanotubes because they sometimes contain frustration in the spin-spin interactions [7,8]. The details are explained in the next section. We investigate the ground state properties of the spin chiral nanotubes with several kinds of chiral vectors.

2. Model

Our model is the spin-1/2 antiferromagnetic Heisenberg tube. The tube is made from a strip of the honeycomb lattice. An example of the strip is shown in Fig. 1. The honeycomb strip can be seen as the coupled dimerized chains in the strongest dimerization limit with the configuration of the dimers in the anti-phase way along the interchain direction. Using the terminology of the low-dimensional strongly correlated systems, we call the bond along the dimerized chains as the ‘leg’ and that along the interchain direction as the ‘rung’. The Hamiltonian is written as follows.

$$
H = J_x \sum_{k=1}^{n} \sum_{j=1}^{L} \left[ \frac{1 + (-1)^{j+k}}{2} \right] S_{j,k} \cdot S_{j+1,k} \\
+ J_y \sum_{j=1}^{L} \left( \sum_{k=1}^{n-1} S_{j,k} \cdot S_{j,k+1} + S_{j,n} \cdot S_{j+1,1} \right)
$$

(1)

Here $S_{j,k}$ is the spin-1/2 operator with $j$ ($k$) specifying the position on the leg (rung). The number of legs is $n$, and the number of sites along the leg is $L$. We impose the periodic boundary condition in both of the rung and the leg directions such that $S_{L+1,k} = S_{1,k}$ and $S_{j,n+1} = S_{j+1,1}$. If $m$ is finite, chirality is introduced in the tube structure. The coupling constants $J_x$ and $J_y$ are positive. We set the $x$-axis along the dimerized chains. The ground state property in the thermodynamic limit, $L \to \infty$, is investigated.

In our spin nanotube, the same structure as that of the carbon nanotube is kept when the imposed periodic boundary condition along the rung direction satisfies the condition that $(n + m)$ is an even number. In this case, there is no frustration between the spin-spin interactions and we can perform numerical experiments by the quantum Monte Carlo method without suffering from the negative sign problem [13]. The chiral vector of the tube is defined by $p \mathbf{a}_1 + q \mathbf{a}_2$, where the lattice vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ are shown in Fig. 1. In terms of our parameters, it is written as $(p,q) = ((m + n)/2, (m - n)/2)$.

![Fig. 1. The lattice on which our model is defined. The arrows $\mathbf{a}_1$ and $\mathbf{a}_2$ are the lattice vectors. We set the coordinate system so that the $x$-axis is horizontal. It is topologically equivalent to the strip of the honeycomb lattice. In this figure, the chiral tube is made so that the two sites encircled by a line are identical, which makes the indices of the chiral tube $(n, m) = (3, 1)$. The definitions of $n$ and $m$ are given in Eq. (1) in the text.](image-url)
3. Method and Results

We determine the quantum critical points of the model and discuss their distribution in our parameter space. The positions of them are specified by the parameter $R \equiv J_y/(J_x + J_y)$ which connects continuously the strong leg coupling limit at $R = 0$ to the strong rung coupling limit at $R = 1$. The phase diagram is drawn on the $R$ axis. We note that the isotropic nanotube is realized on the point $R = 0.5$. The phase boundaries are determined by the expectation value of the Lieb-Schultz-Mattis slow-twist operator [14,15], which is used to detect the bond order specific to the gapped states. For our model, it is defined as follows.

$$z_L = \left\langle \exp \left[ \frac{2\pi i}{L} \sum_{j=1}^{L} \sum_{k=1}^{n} S_{j,k}^z \right] \right\rangle_0$$  \hspace{1cm} (2)

Here $\langle \cdot \rangle_0$ means the expectation value in the ground state. The quantum critical points are given by the thermodynamic limit of the zeros of $z_L$. The observables including $z_L$ are evaluated by the quantum Monte Carlo method with the continuous-time loop algorithm [16], which is actually a finite-temperature algorithm, for several finite sizes. Assuming the Lorentz invariance [17], the temperature $T$ is fixed to the value of $T = 1/L$. The critical point in both of the limits $L, T \to \infty$ i.e. the thermodynamic limit at zero temperature, is determined by the crossing point of $z_L$'s calculated for several $L$'s. An example is shown in Fig. 2 for the chiral nanotube with $(n, m) = (3, 1)$. We can identify the quantum critical point at $R_c = 0.38 \pm 0.01$. Thus determined quantum critical points for several chiral nanotubes are shown in Fig. 3.

4. Discussions

The characteristic of the resultant distribution of the quantum critical points in Fig. 3 is the difference with respect to the parity of the number of the fully dimerized chains, $n$. For the nanotube with even (odd) $n$, the number of the quantum critical points is seen to be $n/2$ ($(n - 1)/2$). This reflects the well-known even-odd effect in the ground state of uniform (i.e. non-dimerized) spin ladders [18,4] that is expected to hold also to the spin tubes without frustration. In this effect, the even-legged uniform systems have an excitation gap while the odd-legged ones do not.

We sum up with a few remarks on the comparison of the spin nanotubes with the carbon ones. We note that $n$ is written in terms of the chiral vector, $(p, q)$, as $n = p - q$. The topology of the ground-state phase diagram of the spin nanotubes is determined by the parity of $n$, in contrast to the carbon nanotubes where the electric property on the point $R = 0.5$ is known by asking whether $(p - q)$ is a multiple of 3 or not. So far we have only determined the quantum critical points of the spin chiral nanotubes and discussed the topology of the ground-state phase diagram with respect to the chiral vector. Further investigations are now in progress.
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