Antichirality and elementary excitations of effectively 2D quantum frustrated antiferromagnetic systems

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An exactly solvable 2D quantum spin model is analyzed. It is shown that elementary excitations carry a nonzero spin chirality (a topological charge), but only pairs of these excitations with opposite chirality contribute to the thermodynamics, so the system is always in an antichiral spin state. It is suggested that the elementary excitations of the quantum antiferromagnet discussed here are massive if there are no topological terms in the Hamiltonian. © *1994 American Institute of Physics.*

Quantum antiferromagnets have reattracted research interest in the last few years, primarily because of Anderson's hypothesis[1] that the behavior of such antiferromagnets is pertinent to high-T_c superconductivity. There is accordingly the important question of whether elementary excitations in 2D quantum antiferromagnets have a gap in their spectrum. Unfortunately, this fundamental question cannot be answered rigorously in approximate descriptions.[2–6] It is thus worthwhile to study quantum spin models which can be solved exactly. Two-dimensional quantum systems are also of interest because they allow the existence of the elementary excitations known as anyons, whose statistics lies between those of the Bose and Fermi cases.[7] Several authors link this feature of 2D quantum systems with the behavior of metal oxides (see Ref. 8, for example). In a well-known paper,[9] Wen and co-workers related superconductivity in strongly correlated electron systems with spin chiral states which break the T and P symmetries of the system.

In this letter we present an exact solution, found by the quantum method of the inverse scattering problem,[10] of the Schrödinger problem for an effectively 2D quantum model spin system in which T and P symmetries are broken. We show that excitations of this system, which are analogous to classical instanton solutions,[11] are gapless. They carry a nonzero spin chirality, but only pairs of these excitations with opposite chirality contribute to the thermodynamics. These systems could accordingly be called "antichiral."

We first consider the very simple case of two spin-1/2 chains in which the basic properties of the 2D space are preserved. The Hamiltonian of the system is

$$H=\sum_n \{8(\mathbf{s}_{1,n}\mathbf{s}_{2,n}+\mathbf{s}_{1,n}\mathbf{s}_{2,n+1})+4\theta^2(\mathbf{s}_{1,n}\mathbf{s}_{1,n+1}+\mathbf{s}_{2,n}\mathbf{s}_{2,n+1}) + 8\theta\epsilon^{ikl}(s^i_{1,n}-s^i_{2,n+1})s^k_{1,n+1}s^l_{2,n}-E_f, \qquad (1)$$

where the operators $s^i_{1,2,n}$ $(i=x,y,z)$ represent the ith projection of the spin on the first or second chain at site n, θ is an interaction parameter, and E_f is the energy of the "ferromagnetic" state. The third term in Hamiltonian (1) is unusual in form. It may stem from a spin–orbit interaction if the orbital motion is frozen at sufficiently low temperatures. In this case θ is proportional to $\langle \epsilon^{ikl}(l^i_{1,n}-l^i_{2,n+1})l^k_{1,n+1}l^l_{2,n}\rangle$, where the operator $l^i_{1,2,n}$ represents the ith projection of the orbital angular momentum of the electron, and the angle brackets mean the expectation value. It can be seen from expression (1) that the third term breaks T and P symmetries individually, while TP symmetry is unbroken. Only the replacement of 1 and 2 and $(n+1)$ by $(n-1)$, and vice versa, leaves the Hamiltonian unchanged. The structure of third term can be understood in the long-wave limit. Denoting by $\mathbf{n}$ the density of the spin ($\mathbf{n}^2=1$), we see that the effect of the third term is analogous (in a phase with a zero magnetic moment):

$$I_0=(\theta/2\pi)\int \epsilon^{ikl}\epsilon_{\mu\nu}n^i\partial_\mu n^k\partial_\nu n^l d^2x, \quad \mu,\nu=1,2. \tag{2}$$

Expression (2) is the definition of the topological (Noether) charge for the chiral field $\mathbf{n}$ or the time component of the conserved topological current. Two $\mathbf{n}$ fields can continuously deform into each other only under the condition[12] $I_{0,1}=I_{0,2}$. In the classical case, we know that (I_0/θ) is an integer[12]—specifically, the number of instantons in the system. In another representation of the $\mathbf{n}$ field, we easily recognize the Chern–Simons term[7] in the third larger term. The Chern–Simons term is specific to (2+1)-dimensional systems. For (1+1) or (3+1), it is not possible to construct a conserved scalar or pseudoscalar with the properties of a topological charge. For (3+1), for example, we have the vector I_α instead of I_0, and we can construct a Hopf invariant which takes on only integer values.[12] In the (2+1) case, I_0 is a characteristic of the homotopy class[13] $\pi_2(S^2)=Z$. The field distribution is topologically nontrivial if $\pi_2(S^2)\neq 0$. This term is a total time derivative[14] $\partial_0 I_0=0$, so it does not alter the classical equations of motion.

From the classical standpoint, frustration occurs in a system with Hamiltonian (1). Two-chain quantum spin models are of practical interest. Several substances with a site spin of 1/2 and with the "triangular" spin–spin interaction discussed above have recently been found.[15]

The equations of the Bethe ansatz for the rapidities λ are[16]

$$\frac{\lambda_j^N(\lambda_j+\theta)^N}{(\lambda_j+i)^N(\lambda_j+\theta+i)^N}=\prod_{\substack{k=1\\k\neq j}}^{M}\frac{\lambda_k-\lambda_j+i}{\lambda_k-\lambda_j-i}, \quad j=1,2,...M. \tag{3}$$

Here N is the number of sites in each chain, and M is the number of spins down. An eigenvalue of the Hamiltonian is

$$E=2\sum_{k=1}^{M}\left[\frac{1}{\lambda_k(\lambda_k+i)}+\frac{1}{(\lambda_k+\theta)(\lambda_k+\theta+i)}\right]. \tag{4}$$

Finding the λ_j from (3), and substituting them in (4), we solve the Schrödinger problem for arbitrary M. In the simple case in which the system has a zero magnetic moment, we have, for the ground state,

$$E_0=-2N\int_{-\infty}^{\infty}d\omega[1+\cos(\omega\theta)][1+\exp|\omega|]^{-1}. \tag{5}$$

Equation (5) is an even function of the chirality parameter θ [we define the spin chirality of the system as the nonzero expectation value of the operator $\Sigma_n\epsilon^{ikl}(e^i_{1,n}-e^i_{2,n+1})\times(e^k_{1,n+1}e^l_{2,n})$. At the same time (as was to be expected on the basis of the classical limit), the ground-state energy is periodic in the parameter θ. In Ref. 16 we called such a state "antichiral."

When a weak magnetic field $h\ll 8(I+2\theta^2)/(1+4\theta^2)$ is applied, we find, using the Wiener–Hopf method,

$$E_0=E_0|_{h=0}-hm^zN+N(\pi m^z/2)^2=E_0|_{h=0}-N(h-\pi)^2. \tag{6}$$

For strong external magnetic fields, $h>8(I+2\theta^2)/(1+4\theta^2)$, the energy of the "ferromagnetic" ground state is $E=-4Nh$. As can be seen from (6), a nonzero magnetic field below the critical value does not alter the antichirality of the system, i.e., the numbers of instantons and anti-instantons. For a very simple doublet excitation we find, following Ref. 17,

$$E_d=E_0+\pi\{\text{sech}(\pi\lambda_0\}+\text{sech}[\pi(\lambda_0+\theta)]. \tag{7}$$

Two doublets can form a singlet or a triplet.[17] It is easy to verify that the doublet state is gapless. The same is true for a singlet and a triplet. The question of a gap in the spin excitations of a 2D spin-1/2 system is of fundamental importance for reaching an understanding of the superconducting and antiferromagnetic orders in metal oxides.[1–6] We have shown here that excitations of a system with Hamiltonian (1) are gapless. However, the Hamiltonian contains topological terms with a θ vacuum.[7] The situation is analogous to the Haldane picture of a 1D antiferromagnet.[18,19] Haldane suggested that chains with an integer site spin have a gap in their spectrum, while excitations in chains with a half-integer spin at the sites are gapless. However, the difference between the descriptions of systems with integer and half-integer site spins is in specifically the term with the θ vacuum: It does not alter the classical equations of motion, but it substantially alters the quantum properties of the system. For systems with half-integer site spins we have $\theta\neq 0$; this condition causes the gap to vanish.[18] Using the same arguments which Haldane employed, we might suggest that in our case a gapless behavior of the excitations of the system stems from the nonzero θ term in Hamiltonian (1). (The spatial anisotropy of the spin–spin interaction, which is proportional to an even power of θ, does not erase the gap in the absence of a topological charge, if we work by analogy with Ref. 19, for example.) It can thus be assumed that a 2D quantum frustrated spin system with a site spin of 1/2, but without a chiral increment in the Hamiltonian, has elementary excitations with a gap. These spin gaps may be a source of an antiferromagnetic "quasi-order,"[2–6] and strongly correlated 2D systems may exhibit superconducting properties,[8] as in Laughlin's picture of the fractional Hall effect.[20] The effect of a magnetic field perpendicular to the plane passing through the chains is also analogous to a topological term (Ref. 21, for example; this term is an effective surface term in spin space). In this case the θ vacuum in the model under study here is analogous to a statistical field of anyons.[7] At values of the external field which cancel the internal θ vacuum, the excitations of the system have a gap, while in other cases they are gapless, and the picture corresponds to the picture of the fractional Hall effect.[7] Another basis for our suggestion is provided by the exact classical solutions for a 2D magnetic material,[21] in which the excitations are massive (see also Ref. 22) and in which the chiral equations of the Bethe ansatz are similar to (2), and for the Wess–Zumino–Novikov–Witten model,[23] in which the excitations are gapless because of the θ-vacuum term.

Double excitations alter the chiral properties of the system, since expression (7) is not even in θ. Analysis shows, however, that the contribution of these excitations (spinons) to the thermodynamics comes from pairs with different chirality signs (like excitations carrying a larger spin). This result of course agrees with the circumstance that the topological charge of a system does not change either when a nonzero external field is applied or at a nonzero temperature.

We have discussed the case of two spin chains in detail. We now generalize the discussion to an arbitrary number of chains. For L (L is an even number) spin-1/2 chains, we have the following expression for the transfer matrix and the Hamiltonian:

$$T(\lambda)=T(\lambda-\theta_1)T(\lambda-\theta_2)...T(\lambda-\theta_L), \tag{8}$$

$$H=-E_f+\sum_{r=1}^{L}\sum_{n}\left\{P_{s_{r,n}s_{r+1,n}}+\left(\prod_{\text{VSE}}\theta_{ik}\right)P_{s_{r,n}s_{r,n+1}}\right.$$
$$\left.+\sum_{p<q}\theta_{pq}^{-1}\left(\prod_{\text{VSE}}\theta_{ik}\right)[P_{s_{p,n}s_{q,n}},(P_{s_{p,n}s_{p,n+1}}+P_{s_{q,n}s_{q,n+1}})]+....\right. \tag{9}$$

Here P is a permutation operator; in the first larger term we need to replace the term $P_{s_{L,n}s_{1,n}}$ by $P_{s_{L,n}s_{1,n+1}}$ (this case corresponds to boundary conditions which wind around a torus); $\theta_{ik}=\theta_i-\theta_k$, $\theta_{L+1k}=\theta_{1,k}$; the products are over all i and k; and $T(\lambda)$ is the standard transfer matrix of one spin-1/2 chain.[10] In the limit $\theta_{ik}\to\infty$ we have L noninteracting chains of N spins. In the limit $\theta_{ik}=0$ we have a chain of LN spins. We have omitted from (9) some higher-order terms with commutators. All of them, like the third term, are of the same nature as in the case of two chains, since they do not alter the classical equations of motion, and they constitute topological charges on a lattice of higher order in terms of spin operators. The terms which have been omitted satisfy the long-range nature of the Chern–Simons term in 2D systems.[7] The energy of a system with M spins down is

$$E=\sum_{r=1}^{L}\sum_{k=1}^{M}\frac{1}{(\lambda_k+\theta_{r1})(\lambda_k+\theta_{r1}+i)}, \tag{10}$$

and the λ_k are found from the system of equations

$$\prod_{r=1}^{L}=\frac{\lambda_j^N(\lambda_j+\theta_{r1})^N}{(\lambda_j+i)^N(\lambda_j+\theta_{r1}+i)^N}=\prod_{\substack{k=1\\k\neq j}}^{M}\frac{\lambda_k-\lambda_j+i}{\lambda_k-\lambda_j-i},\quad j=1,2,...,M. \tag{11}$$

In the limit $N\to\infty$ we have the following expression for the ground state:

$$E_0 = -\sum_{r=2}^{L} N \int_{-\infty}^{\infty} d\omega |1 - \exp(i\omega\theta_{r1}|^2 [1 + \exp|\omega|]^{-1}. \tag{12}$$

For this state we have $M = LN/2$. By analogy with expression (7) we can derive an equation for a spinon excitation:

$$E_d = E_0 + \pi \sum_{r=1}^{L} \text{sech}[\pi(\lambda_0 + \theta_{r1})].$$

As in the case of two chains, only pairs of these excitations with opposite chiralities contribute the thermodynamics, and a 2D quantum system with Hamiltonian (9) is antichiral, although each of the spinon excitations carries a nonzero chirality (a nonzero topological charge). Again in this case, the excitations are gapless. As in the case of two chains, however, the Hamiltonian of this system contains nontrivial topological terms which break the T and P symmetries of the system and which, as before, may be the reason for the absence of a gap. Again by analogy with Haldane's work, we can suggest that a frustrated, quantum, effectively 2D antiferromagnet with site spins of 1/2 has gap excitations.

In summary, we have discussed a frustrated, effectively 2D quantum system whose Hamiltonian breaks T and P symmetries and allows an exact solution. There is a spin antichirality in this system. We have shown that a doublet excitation of this system, which is analogous to classical instantons, carries a nonzero spin chirality, but only pairs of these excitations with opposite chiralities contribute to the thermodynamics. We suggest that the topologically nontrivial terms in the Hamiltonian are responsible for the gapless behavior of excitations in this system. We also believe that the elementary excitations have a gap for frustrated, 2D quantum systems without T and P breaking.

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