Berry phase induced dimerization in one-dimensional quadrupolar systems

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We investigate the effect of the Berry phase on quadrupoles that occur for example in the low-energy description of spin models. Specifically we study here the one-dimensional bilinear-biquadratic spin-one model. An open question for many years about this model is whether it has a non-dimerized fluctuating nematic phase. The dimerization has recently been proposed to be related to Berry phases of the quantum fluctuations. We use an effective low-energy description to calculate the scaling of the dimerization according to this theory, and then verify the predictions using large scale density-matrix renormalization group (DMRG) simulations, giving good evidence that the state is dimerized all the way up to its transition into the ferromagnetic phase. We furthermore discuss the multiplet structure found in the entanglement spectrum of the ground state wave functions.

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How quantum fluctuations melt a classical order and create novel quantum states is a fundamental question of modern condensed matter physics. Among many phenomena, mechanisms involving topological effects have been studied in great detail in one-dimensional spin chains as minimal models. In particular, the Berry phase associated with rotation of spins plays a crucial role, as its presence discriminates between antiferromagnetic Heisenberg chains with half-integer and integer spins, making the excitations in the former gapless and in the latter gapped.

A similar Berry phase appears for the spin quadrupoles (nonmagnetic spin states) we investigate here. The quadrupolar order can be found in a simple SO(3) symmetric $S = 1$ Heisenberg model

$$\mathcal{H} = \sum_{l=1}^{L-1} \cos \theta (S_l \cdot S_{l+1}) + \sin \theta (S_l \cdot S_{l+1})^2,$$

where $\theta$ parameterizes the ratio of the bilinear and biquadratic terms and $L$ is the length of the chain. The phase diagram of this model is shown in Fig. 1(a) [8]. It is generally agreed that the model exhibits a ferromagnetic phase, a gapped "Hal-dane" phase, a gapless trimerized phase and a gapped dimerized phase [9]. A long lasting debate has been going on about the possible existence of a non-dimerized gapped phase above the $\theta_F = -3\pi/4$ SU(3) symmetric point. This phase can be thought of as a nematic phase that has become disordered on account of quantum fluctuations (since the system is one-dimensional). At $\theta_F$ the ground state is degenerate, and it has no fluctuations: any state where each spin is in the same state is a ground state. Slightly away from $\theta_F$, nematic states of the spins have lower energies than other states, so the state will be approximately a uniform state of nematic spins. Due to quantum fluctuations, the order will only last up to the correlation length. There is no obvious reason that this state should become modulated with a period of 2 near this point (there is no minimum in the spin-wave dispersion near $\pi$). Could this be a fifth homogeneous phase between the ferromagnetic and the dimerized phase? This question was first raised in [8], which also calculated that this phase would exist for $\theta_F < \theta \lesssim -0.66\pi$. This idea was supported both theoretically [10] and numerically [11, 12]. Almost at the same time, exact diagonalizations of finite chains [13] provided an indication for the absence of this phase near $\theta_F$, and similar conclusion was reached by a variational study [14] in the context of cold atoms. Despite the progress in numerical techniques, more recent simulations still are producing contradicting results [15].

Refs. [16, 17] found a reason why the nematic phase becomes dimerized, related to Berry phases associated with quantum fluctuations of the quadrupoles, which we will test here. We will find how the dimerization near $\theta_F$ varies using a quantum rotor model, and then calculate the actual dimerization numerically (using the density matrix renormalization group method [18, 19]) to check the prediction. We further explore in detail the entanglement spectrum for which we derive exact expressions at $\theta_F$.

Let us start from the ordered quadrupolar mean-field wave function in the vicinity of $\theta_F$ with $\theta \geq \theta_F$:

$$|\psi_{\text{MF}}\rangle = \prod_{l=1}^{L} |\psi_l\rangle = \prod_{l=1}^{L} (n^x|x\rangle + n^y|y\rangle + n^z|z\rangle),$$

with $n^x, n^y$ and $n^z$ being real numbers. The states $|x\rangle = i(|1\rangle - |\bar{1}\rangle)/\sqrt{2}$, $|y\rangle = (|1\rangle + |\bar{1}\rangle)/\sqrt{2}$ and $|z\rangle = -i|0\rangle$ form the time-reversal invariant basis of the $S = 1$ spins at site $l$ ($|1\rangle$, $|0\rangle$ and $|\bar{1}\rangle$ the $S^z$ eigenstates). Being fully symmetric, $|\psi_{\text{MF}}\rangle$ is an exact ground state at the SU(3) symmetric point $\theta_F$ [20]. The mean-field wave function does not have the full SO(3) symmetry. The order parameter can be thought of as an ellipsoid or rod, as shown in Fig. 1(b). It has a rotational symmetry $\exp(i\gamma \mathbf{\hat{n}} \cdot \mathbf{S})|\psi_{\text{MF}}\rangle = |\psi_{\text{MF}}\rangle$ with any angle $\gamma$ around $\mathbf{n} = \pm (n^x, n^y, n^z)$, as well as an additional $\mathbb{Z}_2$ symmetry from flipping the direction axes $\mathbf{n} \rightarrow -\mathbf{n}$. This
FIG. 1. (color online) (a) Phase diagram of the spin-one Hamiltonian Eq. (1). (b) In the quadrupolar state \( |y \rangle \) the spin fluctuates over the yellow region perpendicular to the director (green) \( |\hat{n} \rangle \)[6,7]. (c) Rotating a director along the blue path in the projective plane will not produce a Berry phase, while after a nontrivial winding (red path) the quadrupole will pick up a \( \pi \) Berry phase. (d) World lines of directors in 1 + 1 dimensional space-time. The directors tend to align with adjacent ones in space (due to the spring constant \( K \)), and they can rotate in time, with a moment of inertia \( I \). Rotations of a director as a function of time lead to a Berry-phase. Directors can either rotate by an angle 0 or \( \pi \) as shown in the two highlighted world lines, picking up a phase \( \pi \) in the latter case. To keep track of the total rotation, we add a red dot onto the green ellipsoid. In between domains of different windings, \( \pi \)-vortices appear (big black dots).

extra symmetry distinguishes the quadrupolar order from the ferromagnetic order. As a consequence, the “director” \( \hat{n} \) lives in the projective plane \( \mathbb{RP}^2 \) formed by identifying antipodal points of the unit sphere \( S^2 \) [Fig. 1(c)].

Because the \( \mathbb{Z}_2 \) symmetry, we can distinguish two topologically distinct classes of closed adiabatic paths of the \( \hat{n} \): the paths can cross the boundary of the \( \mathbb{RP}^2 \) an even or odd number of times [see Fig. 1(b)]. Since the Berry phase for the time reversal invariant quadrupoles is quantized to 0 or \( \pi \) (in contrast to spin coherent states) \([21]\), the phase on homotopic paths will be equal. In the case of 0 or even number of crossings the path can be contracted to a single point, and we expect no Berry phase. For an odd number of crossings the path cannot be contracted, and the wave function can acquire a Berry phase. For a spin-1 quadrupolar state \( |z \rangle \), this phase is \( \pi \). To see this, we rotate the \( |z \rangle \) around the \( y \)-axis by slowly changing \( \varphi = 0 \) to \( \pi \) as \( |\psi(\varphi)\rangle = \cos \varphi |z\rangle + \sin \varphi |x\rangle \). In this gauge the Berry connection \( i\langle \psi(\varphi) | \partial_\varphi |\psi(\varphi)\rangle = 0 \) and the Berry phase is just given by the change of the sign of the wavefunction which is \( -1 \).

On account of the Mermin-Wagner theorem, quantum fluctuations are large enough to cause the state to become disordered. To understand the consequences, we will assume that the low energy fluctuations are described by a rotor model\([10,22]\]

\[
\mathcal{H} = \sum_{l=1}^L \frac{L^2}{2I} - \frac{K}{2} (\hat{n}_l \cdot \hat{n}_{l+1})^2 .
\]

Here the first term is the kinetic energy of the directors (the original spin \( S_l \) and the angular momentum \( L_l = I \hat{n}_l \times \partial_t \hat{n}_l \) coincide when averaged over enough sites), the second term is the \( \mathbb{Z}_2 \) symmetric interaction between two adjacent directors. The energy of a twist in the director and the response to a magnetic field can be calculated both from the rotor model and the original spin model (using the mean-field approximation), and comparing these tell us the spring constant and moment of inertia, \( K = -2 \cos \theta \), and \( I = 1/2(\cos \theta - \sin \theta) \). In the continuum description of the model, we rescale the imaginary time \( t = \tilde{t} \sqrt{T/K} \) so that the action becomes isotropic

\[
S = \frac{1}{2g_0} \int dt dx \left[ (\partial_\tilde{t} \hat{n}(\tilde{t}, x))^2 + (\partial_x \hat{n}(\tilde{t}, x))^2 \right] ,
\]

where the dimensionless stiffness \( 1/g_0 = \sqrt{TK} \).

We now use space-time path integrals to show that, when the Berry phase associated to the \( \mathbb{Z}_2 \) symmetry of Eq. (4) is \( \pi \) (as for the spin-1 case) the ground state becomes dimerized. As illustrated in Fig. 1(d), the \( \hat{n} \) field in the two-dimensional \( (x, \tilde{t}) \) space has topological defects in the form of vortices. Because of the continuous O(3) rotation symmetry \( \hat{n} \) does not have long-range order. Since \( \hat{n} \) has three components, just spin waves lead to exponentially decaying correlations \([23]\) (vortices are not necessary). This causes vortices to have a finite action, so “entropy” produces them at any stiffness, and this will make the entire phase dimerized. That is because the vortices separate domains where worldlines of the directors have different winding numbers (and hence different Berry phases 0 and \( \pi \)). Let us for clarity first assume that we have only one pair of vortices. The sign of the path integral depends on their distance: the sign is positive (negative) if the vortices separate domains where worldlines of the directors are aligned (not aligned) in space. For \( 2N^v \) vortices, the product over all pairs gives the total sign \( \prod_{j=1}^{2N^v} (-1)^{x_j} \), where \( x_j \) are the indices of bonds that vortices live on. This gives rise to a dimerization of the system as path integrals come with opposite signs depending on whether the vortices are located on even or odd bonds relative to each other. From this reasoning, we expect that the dimerization strength \( D \) is proportional to the density of vortices.

Let us now apply this qualitative theory and predict the scaling behaviors of the correlation length and dimerization strength. Based on the fact that the O(3) symmetry is not broken, we find, as noted in Ref. \([23]\), that the renormalized stiffness \( 1/g(r) = 1/g_0 - (\ln r)/2\pi \) decreases for longer length scales (the distance \( r^2 = x^2 + \tilde{t}^2 \)), eventually disappearing for \( r \gtrsim \xi \), where

\[
\xi = \exp \left( 2\pi \sqrt{TK} \right) \approx \exp \left( \pi \sqrt{2/\Delta \theta} \right) ,
\]
and $\Delta \theta = \theta - \theta_F$. The correlations also disappear for $r \gtrsim \xi$. This derivation is very similar to the argument in Ref. [10], up to a factor of two in the exponential.

Supposing that the dimerization is proportional to the density of vortices, we are now able to estimate the dimerization strength quantitatively. For a classical vortex shown in Fig. 2(d), we find that $|\nabla \hat{n}|^2 = 1/4r^2$. To take into account that the size of a vortex is $\xi$, we assume that the stiffness is decreasing gradually from the core of the vortex out to $\xi$, so that the action $S^\theta = \int_r^\xi dr 2\pi r |\nabla \hat{n}|^2 / 2g(r) = (\ln \xi)^2 / 16$. The density of vortices is proportional to $\exp(-S^\theta)$, so the dimerization is

$$D \propto \exp \left( \frac{-\ln^2 \xi}{16} \right) \approx \exp \left( -\frac{\pi^2}{8\Delta \theta} \right).$$

The gap has the same order as $1/\xi \approx \exp(-\pi \sqrt{2/\Delta \theta})$, so the dimerization is much smaller than the gap close to $\theta_F$. This is very different than usual spin density waves, where the gap is proportional to the dimerization. In an ordinary system with a spin density wave, the dimerization leads to scattering between the two edges of the Fermi surface which causes a gap. The gap is proportional to the amount of scattering, which is proportional to the difference in the potential at the even and the odd bonds.

We will now compare expressions (5) and (6) with numerical DMRG simulations [18]. The correlation length is obtained by diagonalizing the transfer matrix [24] and the dimerization strength is defined as $D = |E_s - E_w|$ with $E_s$ ($E_w$) being the energy on strong (weak) bonds. In order to reach sufficiently large system size, we use an improved DMRG technique with open boundary conditions [19]. We performed simulations with different numbers of kept states up to $m \leq 4000$ for system sizes up to $L = 20000$ and extrapolate to the $m \to \infty$ limit where needed. Our results, shown in Fig. 2 confirm the scaling behavior of both the correlation length and the dimerization strength (the open chain dimerizes) predicted by the effective field theory in the vicinity of $\theta_F$. Based on numerical simulation we conclude that the low-energy (i.e., long wave-length) behavior is described by the rotor model together with Berry phases, yielding a gapped and dimerized phase up to the transition to the ferromagnetic phase.

After focussing on the physics at long distances, we will now also consider shorter length scales. We find the three different regions shown in Fig. 3. The bipartite spin fluctuations are given by $F = \langle (S^\theta_R)^2 \rangle$ [25] and the $S_E$ is the von Neumann entropy of the reduced density matrix $\rho_L$. Both quantities are calculated for the bipartition of a chain of length $L$ into two (left, $L$, and right, $R$) half chains of equal length. At short and intermediate distances, the ground state appears to be critical. In particular, the entanglement entropy $S_E$ shows a logarithmic growth as a function of system size. This is a known hallmark of conformally invariant, critical systems for which $S_E = (c/6) \log L$ with $c$ being the central charge, i.e., the number of linearly dispersing modes [26, 27].
our system is not conformally invariant, we still use the notation of $c$ to characterize the behavior at shorter length scales. The short distance region is described by an effective $c = 6$ and the bipartite fluctuations $\mathcal{F}$ grow linearly with the system size (green lines). Both properties are inherited from the exactly soluble SU(3) point (see discussion below). Above a scale $L_{\text{m}} \propto \sqrt{\Delta \theta}$, the magnetic healing length, but below $\xi$, the critical behavior changes to an effective $c = 2$ and a logarithmic growth of $\mathcal{F}$ (yellow lines), because there are two approximate Goldstone modes of the rotors $\theta_{F}$. For sufficiently large sizes $L \gg \xi$ the growth of the entropy is cut off by the gap and the fluctuations saturate (red lines). The fact that the correlation length $\xi$ is of the order of thousands of sites in the scaling regime near $\theta_{F}$ might explain why previous numerical studies predicted a critical phase instead of a dimerized one.

For a number of different systems it was shown that conclusive information about a state can be extracted from the entanglement spectrum $\rho_{S}$. The set of eigenvalues $\{\rho_{1}\}$ of the reduced density matrix $\rho_{S}$. Figures 3(a) and (b) show the spectrum as a function of $\Delta \theta$ for the two inequivalent bonds. The apparent multiplet structure reflects the SO(3) symmetry of the state. The lowest levels have the same multiplicities as in a perfectly dimerized state, where cutting a strong bond gives a three fold degenerate state as we cut a spin-1 singlet, while cutting a weak bond gives a non-degenerate state. In the limit $\theta \to \theta_{F}$ we can actually derive an exact expression for the entanglement levels. The $2S_{L} + 1$ degenerate eigenvalues of the corresponding reduced density matrix $\rho_{S}$ for a bipartition into two half-chains are

$$
\rho_{S_{L}}(L, \theta_{F}) = \frac{[2S_{L} + 1]![(L/2+S_{L})/2]!}{[(L/2+S_{L}+1)!((L/2-S_{L})/2)!]} \cdot (7)
$$

where the allowed total spins $S_{L}$ are even for $L/2$ even, while they are odd for $L/2$ odd $S_{L}$. [Figs. 3(a) and (b)]. The observed short-range behavior in Fig. 3 is readily reproduced using Eq. (7), we get $S_{L}/\ln L \to 1$ and $\mathcal{F}/L \to 1/6$ as $L \to \infty$.

As we move away from the $\theta = \theta_{F}$, additional states appear in the entanglement spectrum (grey levels in Fig. 4). Since the ground state is SO(3) symmetric, we can plot the entanglement spectrum as a function of $S_{L}(S_{L}+1)$, Figs. 4(c) and (d). The lower edge of the spectrum graphed in this way is linear, similar to the Anderson tower found for the energy spectra of ordered spin systems $\mathcal{F}$. The presence of every other spin only is typical for a ferroquadrupolar phase (Anderson towers in entanglement spectra have also been discussed in $\mathcal{F}$-value). Unlike for gapless systems, the linear slope $A_{1}$ of the Anderson tower remains finite. Its states contribute roughly $1/A_{1}$ to the spin fluctuation of an infinite half-chain $\mathcal{F}$.

Thus we can estimate $A_{1}$ from the bipartite spin fluctuations if we assume other states do not change the order of magnitude of the spin fluctuations. The spin correlation function is given by $G^{s}(x) = -(1/2\pi)^{2}\ln(\xi/x)/x^{2}$, so the bipartite spin fluctuations are $\mathcal{F} = \int_{0}^{\pi} dx_{0} \xi_{0}^{-2} - \xi_{0}^{2} \xi_{0}^{2} \ln^{2} \xi_{0}^{2}$ in the leading order. Thus we expect $1/A_{1} \propto \ln^{2} \propto 1/\Delta \theta$, and this agrees with the numerical results shown in Fig. 4(c) when $L \gg \xi$, though the anticipated behavior is reached only in the asymptotic limit as indicated in Fig. 4(f).

In this manuscript, we studied the effect of the Berry phase on quadrupoles that occur in the effective description of the one-dimensional bilinear-biquadratic spin-one model. From the effective low-energy theory, we showed that quantum fluctuations melt the nematic order to produce a gapped state, while vortices and a Berry phase cause dimerization. The scaling predicted by this theory was verified using large scale density-matrix renormalization group simulations. Additional insight into the nature of the ground state was obtained by studying the entanglement spectrum. Beyond magnetic systems, our findings are of relevance to cold spin one bosons, where dimerization would occur quite naturally $\mathcal{F}$.
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$$\mathcal{F} = \frac{\sum_{S^z_\mathbf{L}} (2S^z_\mathbf{L} + 1)S^z_\mathbf{L} S^z_\mathbf{L} + 1 \exp (-A_1 S^z_\mathbf{L} S^z_\mathbf{L} + 1))}{3 \sum_{S^z_\mathbf{L}} (2S^z_\mathbf{L} + 1) \exp (-A_1 S^z_\mathbf{L} S^z_\mathbf{L} + 1))} \approx \frac{1}{3A_1}$$

as $\theta \to \theta_F$. This follows from the fact that the total of all the spins is zero, because it implies that $\langle S^z_\mathbf{L}^4 \rangle = -\langle S^z_\mathbf{L}^2 \rangle$, which can be expanded as a sum of $G^2 (x-y)$. To get a rough estimate, one can stop the sums when $|x-y| > \xi$. 

\[ \]