



Path integral for spin-1 chain in the fluctuating matrix product state basis

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An alternative method of writing down the path integral for spin-1 Heisenberg antiferromagnetic chain is introduced. In place of the conventional coherent-state basis that leads to the nonlinear σ model, we use a basis called the fluctuating matrix product states which embodies intersite entanglement from the outset. It forms an overcomplete set spanning the entire Hilbert space of the spin-1 chain. Saddle-point analysis performed for the bilinear-biquadratic spin model predicts the Affleck-Kennedy-Lieb-Tasaki (AKLT) state as the ground state in the vicinity of the AKLT Hamiltonian. Quadratic effective action derived by gradient expansion around the saddle point is free from constraints that plagued the nonlinear σ model and exactly solvable. The obtained excitation modes agree precisely with the single-mode approximation result for the AKLT Hamiltonian. Excitation spectra for other bilinear-biquadratic Hamiltonians are obtained as well by diagonalizing the quadratic action.

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The coherent-state representation of spins is a vital component in constructing the path integral of the spin Hamiltonian. It is defined as the eigenstate satisfying $(\mathbf{S} \cdot \mathbf{n})|\mathbf{n}\rangle = |\mathbf{n}\rangle$, where \mathbf{n} refers to the classical spin orientation and \mathbf{S} is the spin operator. For multispin problems the coherent-state basis becomes a direct product $\prod_i |\mathbf{n}_i\rangle = |\mathbf{n}_1\rangle \otimes |\mathbf{n}_2\rangle \otimes \dots$ over all the sites of the lattice, i . Such basis offers an intuitive mapping of the spin Hamiltonian to the path-integral form, accomplished by replacing each spin operator by its classical counterpart $\mathbf{S}_i \rightarrow S\mathbf{n}_i$ (S =spin size). The Berry phase action arises naturally in the coherent-state representation as $\sum_i \langle \partial_t \mathbf{n}_i | \mathbf{n}_i \rangle = -iS \sum_i (1 - \cos \theta_i) \partial_t \phi_i$, as the sum over all spin variables, in the spherical coordinates $\mathbf{n}_i = (\sin \theta_i \cos \phi_i, \sin \theta_i \sin \phi_i, \cos \theta_i)$ [1]. Haldane argued that this Berry phase leads to a topological action which can critically affect the spin dynamics depending on the parity of the integer $2S$ [2]. The essence of the spin-1 antiferromagnetic chain problem is captured in a crisp manner by the Affleck-Kennedy-Lieb-Tasaki (AKLT) model Hamiltonian and its exact ground state [3,4]. Later work showed how to cast the AKLT state as a matrix product state (MPS) [5]. More recent developments, mostly taking on the nature of heavy numerics, are on the investigation of the dynamics of the integer spin chain by enlarging the MPS scheme to encompass low-lying excited states [6–8].

We present a path-integral approach to the integer spin chain model. The idea is to employ, instead of the product of site-based coherent states of spins, an entangled, MPS-type basis and develop path integrals therein. This is accomplished by generalizing the MPS formalism to include fluctuating correlated states of spins we call the fluctuating MPS (fMPS). The fMPS states are proven to span the entire Hilbert space of the spin-1 chain and satisfy the completeness relation. Using such fMPS basis, the path integral for the spin-1 bilinear-biquadratic (BLBQ) model is constructed following

Feynman's canonical prescription. A related, yet much broader scheme of the MPS-based path-integral approach for spin systems was advanced several years earlier [9]. The approach we initiate here is particularly suited to the spin-1 chain by contrast. Several key differences between our formulation and that of Ref. [9] will be pointed out.

We begin by introducing a singlet bond operator \mathcal{S}_i^\dagger and three triplet bond operators $(\mathcal{T}_i^x)^\dagger$, $(\mathcal{T}_i^y)^\dagger$, and $(\mathcal{T}_i^z)^\dagger$ defined on a pair of adjacent sites $(i, i+1)$ in the Schwinger boson (SB) representation:

$$\begin{aligned} \mathcal{S}_i^\dagger &= \frac{1}{\sqrt{2}}(a_i^\dagger b_{i+1}^\dagger - b_i^\dagger a_{i+1}^\dagger), \\ (\mathcal{T}_i^x)^\dagger &= \frac{1}{\sqrt{2}}(a_i^\dagger a_{i+1}^\dagger - b_i^\dagger b_{i+1}^\dagger), \\ (\mathcal{T}_i^y)^\dagger &= \frac{i}{\sqrt{2}}(a_i^\dagger a_{i+1}^\dagger + b_i^\dagger b_{i+1}^\dagger), \\ (\mathcal{T}_i^z)^\dagger &= \frac{1}{\sqrt{2}}(a_i^\dagger b_{i+1}^\dagger + b_i^\dagger a_{i+1}^\dagger). \end{aligned} \quad (1)$$

Each boson a_i^\dagger and b_i^\dagger creates a spin-1/2 particle of up and down orientations, respectively, at the site i . Notations for the basis operators \mathcal{S}_i^\dagger , $(\mathcal{T}_i^x)^\dagger$, $(\mathcal{T}_i^y)^\dagger$, and $(\mathcal{T}_i^z)^\dagger$ will be used interchangeably with $(N_i^1, N_i^2, N_i^3, N_i^4)$, respectively. The celebrated AKLT ground state is given simply by the product of singlet bond operators $\prod_i \mathcal{S}_i^\dagger$ acting on the SB vacuum $|v\rangle$. In fact, every bond-product state of the form $N_1^{\alpha_1} N_2^{\alpha_2} \dots N_N^{\alpha_N} |v\rangle$, with α_i 's taking one of the four possibilities in Eq. (1) on a closed chain of length N , represents a viable many-body $S=1$ spin state. They also span the entire 3^N -dimensional space of the spin-1 chain [10].

The SB formalism suggests a way to conveniently express excited states of the spin-1 chain, by writing each bond state as a superposition of the four bond operators introduced in Eq. (1). To be concrete, the bond operator N_i (without the upper index) over the $(i, i+1)$ bond as well as the overall

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many-body state $|\mathbf{N}\rangle$ can be introduced as

$$N_i = \sum_{\alpha=1}^4 z_i^\alpha N_i^\alpha, \quad |\mathbf{N}\rangle = \left(\prod_i N_i \right) |v\rangle. \quad (2)$$

One can normalize the complex-valued coefficients $z_i^{\alpha i}$ according to $\sum_{\alpha=1}^4 z_i^\alpha \bar{z}_i^{\alpha i} = 1$ ($\forall i$), where $\bar{z}_i^{\alpha i}$ is the complex conjugate of $z_i^{\alpha i}$. In analogy to the coherent state of spins, we call the above the bond coherent state. Our goal is to develop a path-integral theory of the spin chain within the framework of bond coherent states given in Eq. (2). In particular, we want to focus on the spin-1 BLBQ model that contains both the Heisenberg and the AKLT Hamiltonians as special cases. It is given by $H_{\text{BLBQ}} = \sum_i H_i$ where each H_i is [11–13]

$$\begin{aligned} H_i &= \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \tan \tau (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 \\ &= 1 + \tan \tau - (1 + 2 \tan \tau) S_i^\dagger S_i + \tan \tau (S_i^\dagger S_i)^2. \end{aligned} \quad (3)$$

The bond singlet operator S_i^\dagger [Eq. (1)] is used in the second equality. The Heisenberg and the AKLT Hamiltonians are found at $\tau = 0$ and $\tau_0 \equiv \tan^{-1}(1/3)$, respectively. Note that our formulation does not make explicit use of the so-called tangent-space formulation, developed in Refs. [6–8] and extensively adopted in Ref. [9]. A thorough comparison of the two formulations remains in order. In this Rapid Communication, we focus on the consistent development of the path-integral scheme based on the bond operator formalism starting with Eq. (2).

An essential ingredient in the path-integral construction is the existence of a complete set of continuously varying states $|\mathbf{N}\rangle$ satisfying the completeness relation $\int [\mathcal{D}\mathbf{N}] |\mathbf{N}\rangle \langle \mathbf{N}| \propto I$ over a suitable integration measure $[\mathcal{D}\mathbf{N}]$. In the Supplemental Material (SM) [16] we present proof that $|\mathbf{N}\rangle$ defined in Eq. (2) provides such a complete set, over the space of complex-valued coefficients satisfying the constraint $\sum_\alpha |z_i^\alpha|^2 = 1$. An appropriate integration measure for such CP^3 fields can be found as [14]

$$\begin{aligned} z^1 &= \cos \chi \cos \xi, \\ z^2 &= e^{i\varphi^x} \cos \chi \sin \xi, \\ z^3 &= e^{i\varphi^y} \sin \chi \cos \eta, \\ z^4 &= e^{i\varphi^z} \sin \chi \sin \eta. \end{aligned} \quad (4)$$

Here the ranges of angles are φ^α ($\alpha = x, y, z$) $\in [0, 2\pi]$, $\chi \in [0, \frac{\pi}{2}]$, $\xi \in [0, 2\pi]$, and $\eta \in [0, 2\pi]$. The integration measure for the i th bond variables is

$$\begin{aligned} \int d\Omega_i &= \frac{1}{8\pi^5} \int_0^{2\pi} d\varphi_i^x \int_0^{2\pi} d\varphi_i^y \int_0^{2\pi} d\varphi_i^z \\ &\times \int_0^{2\pi} d\xi_i \int_0^{2\pi} d\eta_i \int_0^{\pi/2} d\chi_i \sin 2\chi_i. \end{aligned} \quad (5)$$

Denoting $[\mathcal{D}\mathbf{N}] = \prod_i d\Omega_i$, the desired completeness relation follows as

$$\int [\mathcal{D}\mathbf{N}] |\mathbf{N}\rangle \langle \mathbf{N}| = I_{3^N \times 3^N}. \quad (6)$$

Details of the proof are in the SM [16]. The completeness proof presented here is in the specific context of bond operator

parametrization with CP^3 fields. A different parametrization of the MPS fields is possible [9,15].

Having found a complete set in the fMPS basis as provided by the bond coherent states $|\mathbf{N}\rangle$, we can follow Feynman's prescription in constructing the path integral by evaluating the time evolution amplitude over an infinitesimal time interval Δt :

$$\begin{aligned} &\frac{\langle \mathbf{N}(t + \Delta t) | e^{-i\Delta t H} | \mathbf{N}(t) \rangle}{\langle \mathbf{N}(t) | \mathbf{N}(t) \rangle} \\ &\simeq \exp \left(i\Delta t \left[-i \frac{\langle \partial_t \mathbf{N}(t) | \mathbf{N}(t) \rangle}{\langle \mathbf{N}(t) | \mathbf{N}(t) \rangle} - \frac{\langle \mathbf{N}(t) | H | \mathbf{N}(t) \rangle}{\langle \mathbf{N}(t) | \mathbf{N}(t) \rangle} \right] \right), \end{aligned} \quad (7)$$

with $|\mathbf{N}(t)\rangle$ denoting the bond coherent state [Eq. (2)] at time t . Each term in the action requires evaluation of the overlap of one many-body state $|\mathbf{N}\rangle$ with another state, e.g., $|\partial_t \mathbf{N}\rangle$, $H|\mathbf{N}\rangle$. In general this is a formidable problem, circumvented in the usual path-integral approach only by use of the product state basis in which the intersite correlations are absent. The employment of product basis states implies that intricate correlations inherent in the model remain “hidden” in the action, demanding a lot of analysis of the resulting action to uncover them. By introducing correlated basis from the start, as we do with the fMPS basis, one can hope that many of the correlations in the model have already been built in, resulting in the effective action that is simple to analyze. Such seems to be the case with the spin-1 chain problem.

The process begins by identifying the lowest-energy configuration in the variational space of fMPS. The spin-1 BLBQ Hamiltonian [Eq. (3)] has the expectation value

$$E = \sum_i \frac{\langle \mathbf{N} | H_i | \mathbf{N} \rangle}{\langle \mathbf{N} | \mathbf{N} \rangle} \quad (8)$$

for some fMPS state $|\mathbf{N}\rangle$. Anticipating a more or less uniform variational state to give the lowest energy, we first search the space of fMPS where each bond operator $N_i = \sum_\alpha z_i^\alpha N_i^\alpha$ is uniform (site independent). One can further invoke rotational symmetry within the triplet space to confine the search only to the (N^1, N^4) sector, parametrized by $z^1 = \cos \frac{\theta}{2}$, $z^4 = e^{i\phi} \sin \frac{\theta}{2}$. For this class of uniform MPS we find $z^1 = 1$ gives the lowest energy $E = -4/3$. This is nothing but the AKLT state in the MPS form. Our variational search is limited to the range of parameters in the BLBQ model $-\pi/4 < \tau < \pi/4$ where the ground states are known to be gapped and paramagnetic [11–13].

The other type of fMPS ansatz investigated assumes uniform singlet, but staggered triplet configuration according to $N_i = z^1 N^1 + (-1)^i z^4 N^4$. The triplet amplitude alternates in sign from bond to bond. In this case, the energy-minimizing state is found at $z^2 = \text{real}$, with the finite mixing angle θ_s as shown in Fig. 1(a). This is a symmetry-breaking state, as evidenced by explicit calculations showing $\langle S_i^x \rangle = \langle S_i^y \rangle = 0$ but $\langle S_i^z \rangle = -\langle S_{i+1}^z \rangle \neq 0$. A plot of $\langle S_i^z \rangle$ for the staggered variational MPS state is presented in the SM for completeness. In fact, one can prove $|S_i^z| = 1$ at the mixing angle $\theta = \pi/2$. The appearance of a magnetic ground state is an artifact of the variational calculation and runs counter to the well-known result that only paramagnetic ground states exist for the BLBQ Hamiltonian for $-\pi/4 < \tau < \pi/4$. To make further analysis possible, we will henceforth confine our attention

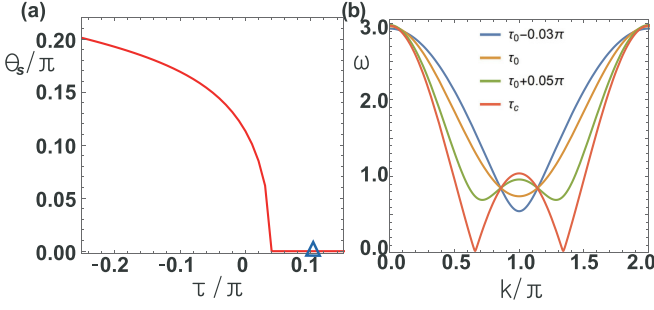


FIG. 1. (a) Mixing angle θ_s at the saddle point of the energy vs the angle τ in the BLBQ Hamiltonian. $\theta_s = 0$ is the AKLT state. The AKLT Hamiltonian is found at $\tau_0 = \tan^{-1} \frac{1}{3}$, indicated by the blue triangle. (b) Dispersion relation obtained from the effective action at various values of τ . An adjustment $k \rightarrow k + \pi$ was made in the formula, Eq. (15), to have our plot agree with other plots of the excitation spectra in the literature. The energy minimum occurs away from $k = \pi$ as $\tau > \tau_0$ and becomes zero at $\tau = \tau_c$ (see text for details).

to $0.04\pi \lesssim \tau < \pi/4$ for which the variational minimum is indeed found at $\theta_s = 0$ (AKLT state) [see Fig. 1(a)]. The painstaking identification of the saddle-point MPS state for the BLBQ Hamiltonian is the foundation for what follows in terms of the fluctuation analysis. A similar spirit of the saddle-point analysis was pursued in Refs. [9,15], but the final effective action they obtain differs from ours.

Effective action can be derived by computing the various overlaps in Eq. (7) for small fluctuations around the AKLT saddle point. In general, this is a highly nontrivial task, as overlaps of many-body states are involved in the computation. Thanks to the well-known gapped spectrum of the AKLT-type ground state, however, we may reasonably anticipate that fluctuations are dominated by the creation of broken singlet bonds, or solitons. Here the solitons are the three triplet bonds [Eq. (1)] taking the place of the singlet bond in the AKLT state. Assuming a low-energy manifold dominated by 0, 1, or 2 solitons in the whole chain, we express the general fMPS states as an expansion in the number of solitons,

$$\begin{aligned} |\mathbf{N}\rangle &\approx \prod_i \left(N_i^1 + \sum_{\alpha=2}^4 (-1)^i z_i^\alpha N_i^\alpha \right) |v\rangle \\ &\approx |A\rangle + \sum_i |\mathcal{T}_i\rangle + \sum_{j<i} |\mathcal{T}_j \mathcal{T}_i\rangle + \dots \end{aligned} \quad (9)$$

The staggered sign $(-1)^i$ introduced in the first line allows a smooth expression of the effective action, without the alternating sign. Smallness of the triplet amplitudes $|z_i^\alpha| \ll 1$ assumes that we are expanding the action around the AKLT saddle point denoted by $|A\rangle$. A one-soliton state is written as $|\mathcal{T}_i\rangle$ and given by replacing the singlet bond operator \mathcal{S}_i^\dagger in the AKLT state by triplet creation operator $\mathcal{T}_i^\dagger = \sum_{\alpha=2}^4 (-1)^i z_i^\alpha N_i^\alpha$. Similarly, $|\mathcal{T}_i \mathcal{T}_j\rangle$ is obtained by introducing a pair of triplet creation operators at $(i, i+1)$ and $(j, j+1)$ bonds. Effective action can be derived by evaluating the overlaps in the path integral (7) systematically up to second power in z_i^α 's. For consistent implementation of the staggered bond factor $(-1)^i$ on a closed chain we adopt even N for the size of the chain.

With abbreviations $\eta \equiv 1/3$ and $f_{ij} = \eta^{|i-j|} + \eta^{N-|i-j|}$, one can prove (see SM at [16] for computational details)

$$\begin{aligned} \langle \mathbf{N} | \mathbf{N} \rangle &= \left(\frac{3}{2} \right)^N \left[1 + \sum_{i,\alpha} |z_i^\alpha|^2 + 2 \sum_{i \neq j, \alpha} f_{ij} x_i^\alpha x_j^\alpha \right], \\ \langle \partial_t \mathbf{N} | \mathbf{N} \rangle &= \left(\frac{3}{2} \right)^N \sum_{i,j,\alpha} f_{ij} (\partial_t \bar{z}_i^\alpha) z_j^\alpha. \end{aligned} \quad (10)$$

We break up the complex coefficients $z_i^\alpha = x_i^\alpha + iy_i^\alpha$ as real and imaginary parts. The ‘‘Berry phase’’ term follows as

$$-i \frac{\langle \partial_t \mathbf{N} | \mathbf{N} \rangle}{\langle \mathbf{N} | \mathbf{N} \rangle} = -i \sum_{i,j,\alpha} f_{ij} (\partial_t \bar{z}_i^\alpha) z_j^\alpha. \quad (11)$$

Different spin orientations α do not mix in the effective action in observance of the rotational symmetry in the space of triplet excitations. Note that $f_{ij} \neq 0$ for $i \neq j$ leads to an unusual, long-ranged Berry phase action in distinct comparison to the coherent-state-based action involving only the local terms $-i \sum_i (\partial_t \bar{z}_i) z_i$. While the z_i 's are $\mathbb{C}\mathbb{P}^1$ fields in the conventional representation of the Berry phase action with constraints $|z_i|^2 = 1$, our fields z_i^α do not have such constraints except that they are small in amplitudes. In other words, z_i^α 's are ‘‘free’’ fields, which make the subsequent calculations easy to handle. The long-ranged part of the Berry phase was not captured previously [9,15] but as one will see, plays a crucial role in deriving the correct dynamics of the BLBQ model.

Energy functional $E_i = \langle \mathbf{N} | H_i | \mathbf{N} \rangle / \langle \mathbf{N} | \mathbf{N} \rangle$ can be worked out in the similar approximation scheme (details are in the SM):

$$\begin{aligned} E_i &= -\frac{4}{3} + 2 \tan \tau + \frac{8}{9} (2 - \tan \tau) \sum_{\alpha} |z_i^\alpha|^2 \\ &\quad - \frac{32}{3} (1 - 3 \tan \tau) \left(\sum_{j < k < i, i < j < k} \eta^{N-|j-k|} + \sum_{j < i < k} \eta^{|j-k|} \right) \\ &\quad \times \sum_{\alpha} x_j^\alpha x_k^\alpha. \end{aligned} \quad (12)$$

Although somewhat lengthy, this is still a quadratic action in terms of free and independent fields z^α and easily diagonalizable. The expression becomes remarkably simple at the AKLT point $\tau_0 = \tan^{-1}(1/3)$ as all the long-ranged interaction terms in the second line vanish.

Equation of motion follows readily from varying the Berry phase action (11) and the total energy $\sum_i E_i$:

$$\begin{aligned} \sum_j (\eta^{|j-i|} + \eta^{N-|j-i|}) \dot{x}_j^\beta - \frac{8}{9} (2 - \tan \tau) y_i^\beta &= 0, \\ \sum_j (\eta^{|j-i|} + \eta^{N-|j-i|}) \dot{y}_j^\beta + \frac{8}{9} (2 - \tan \tau) x_i^\beta \\ &= \frac{8}{3} (1 - 3 \tan \tau) \sum_{j \neq i} F_{i,j} x_j^\beta, \end{aligned} \quad (13)$$

where $F_{i,j}$ is defined as

$$F_{i,j} = 2[(|j-i|-1)\eta^{|j-i|} + (N-|j-i|-1)\eta^{N-|j-i|}].$$

Each triplet branch $\alpha = 2, 3, 4$ acts independently. The equation of motion in the Fourier space, $x_j^\alpha = \sum_{k,\omega} X_{k,\omega}^\alpha e^{ikj-i\omega t}$, $y_j^\alpha = \sum_{k,\omega} Y_{k,\omega}^\alpha e^{ikj-i\omega t}$ gives [omitting spin indices α and (k, ω)]

$$i\omega G(k)X = -\frac{8}{9}(2 - \tan \tau)Y,$$

$$i\omega G(k)Y = \frac{8}{9}[2 - \tan \tau + 3(3 \tan \tau - 1)F(k)]X, \quad (14)$$

where $F(k)$, $G(k)$ are

$$F(k) = \sum_{j \neq i} F_{i,j} e^{ik(j-i)} = \frac{9 \cos 2k - 6 \cos k + 1}{(5 - 3 \cos k)^2},$$

$$G(k) = \sum_j (\eta^{|j-m|} + \eta^{-|j-m|+N}) e^{ik(j-i)} = \frac{4}{5 - 3 \cos k}$$

after taking the large- N limit. After all, ω becomes

$$\omega = \frac{8\{(2 - \tan \tau)[2 - \tan \tau + 3(3 \tan \tau - 1)F(k)]\}^{1/2}}{9G(k)}. \quad (15)$$

Plots of the dispersion for several values of τ are shown in Fig. 1(b). The choice of τ in plotting the dispersion is necessarily confined to the region where the variational MPS ground state equals the nonmagnetic AKLT state, i.e., $\theta_s = 0$ in Fig. 1(a). The well-known single-mode approximation for the excitation energy in the AKLT model is perfectly recovered by the above dispersion formula at $\tan \tau = 1/3$: $\omega(k) = (10/27)(5 - 3 \cos k)$. It differs from the conventional expression $(5/27)(5 + 3 \cos k)$ [17] only due to the fact that our definition of the AKLT Hamiltonian is twice that of the conventional one, and the origin of momentum has been displaced by π due to the staggered factor $(-1)^i$ we used in the gradient expansion, Eq. (9). The dispersion formula derived in Eq. (15) goes beyond the AKLT point and captures the excitation spectrum for a family of BLBQ models. It is also worth noting

that the structure factor $G(k)$, which dominates the dispersion at the AKLT point, entirely comes from the structure of the Berry phase action, having nothing to do with the form of the energy functional. Our dispersion formula becomes gapless at $\tau = \tan^{-1} \frac{23}{37} \approx 0.177\pi$, $k = \pi - \cos^{-1} \frac{13}{27} \approx 0.660\pi$ while the actual BLBQ model becomes gapless at $\tau = \pi/4$ and $k = 2\pi/3$. Such discrepancy is expected given the simple nature of our MPS ansatz. Nevertheless it is nontrivial that a gapless point occurs in our approach at values that are in fair proximity to the exact values. Low-energy modes of the BLBQ Hamiltonian have been worked out elsewhere using extensive numerical methods, e.g., see Fig. 3 in Ref. [7]. Minimum of the dispersion occurs away from $k = \pi$ as τ increases beyond the AKLT value τ_0 , in agreement with the behavior exhibited by our dispersion formula, Eq. (15).

The low-energy effective action for the spin-1 BLBQ Hamiltonian derived here differs from the conventional one built out of spin coherent states. Rather than the CP^1 fields or the classical unit-length vectors governed by the Wess-Zumino action, the set of triplet fields in our action are “free” and has the unusual form involving long-ranged coupling of the fields. Such action did not appear in the earlier MPS formulation either [9,15]. The systematic expansion scheme we develop here of the effective action in terms of small triplet amplitudes proves to be an effective way to derive the effective action in the vicinity of the MPS saddle point. Unraveling the technical differences of our scheme to the tangent-space formulation [9,15] remains.

Note added. Recently, a different kind of path-integral construction using the squeezed states was advanced [18] and applied to study the dynamics of cold atoms.

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