

Path integrals for dimerized quantum spin systems

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Abstract

Dimerized quantum spin systems may appear under several circumstances, e.g. by a modulation of the antiferromagnetic exchange coupling in space, or in frustrated quantum antiferromagnets. In general, such systems display a quantum phase transition to a Néel state as a function of a suitable coupling constant. We present here two path-integral formulations appropriate for spin $S = 1/2$ dimerized systems. The first one deals with a description of the dimers degrees of freedom in an $SO(4)$ manifold, while the second one provides a path-integral for the bond-operators introduced by Sachdev and Bhatt. The path-integral quantization is performed using the Faddeev–Jackiw symplectic formalism for constrained systems, such that the measures and constraints that result from the algebra of the operators is provided in both cases. As an example we consider a spin-Peierls chain, and show how to arrive at the corresponding field-theory, starting with both an $SO(4)$ formulation and bond-operators.

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1. Introduction

Dimerized quantum spin systems appear frequently in quantum antiferromagnets, leading to a spin-liquid in the form of a valence-bond solid (VBS) for strong enough dimerization. A well-known example is given by spin-Peierls systems, where in quasi one-dimensional materials the dimerization can arise due to electron–phonon interaction [1,2]. Dimerized systems constitute also a starting point to study frustrated quantum antiferromagnets in two dimensions.

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In such a way, models with antiferromagnetic exchange interactions beyond nearest neighbors were addressed [3], finding spin-Peierls states, as were suggested from topological events in $SU(N)$ extensions of quantum antiferromagnets [4,5]. Dimerized states also result from frustrating longer-range interactions as in the case of the Shastry–Sutherland model [6], where nearest neighbor (J) and next-nearest neighbor (J') interactions on alternating plaquettes lead to a VBS for large enough values of J'/J ($J'/J \geq 1$ in the isotropic case for spin $S = 1/2$ and in the absence of a magnetic field). In all the cases above, a quantum phase transition (QPT) between a Néel state or some other intermediate state, and a VBS sets in by varying the ratio of the competing couplings. In particular, in the case of the Shastry–Sutherland model, several intermediate phases between the Néel state and the VBS were proposed [7–10]. However, the nature of the intermediate phase is still not clear [11–14].

Two-dimensional dimerized quantum antiferromagnets were also discussed recently [15,16] in connection to the proposal of deconfined quantum criticality [17]. In this theory, the critical point is characterized by the deconfinement of new degrees of freedom resulting from fractionalization of the order parameter, as opposed to the Landau–Ginzburg–Wilson (LGW) paradigm of phase transitions, where the critical point is characterized solely by the critical behavior of the order parameter and its correlators. Specifically, the theory by Senthil et al. [17] allows for a continuous phase transition between a Néel state, that breaks rotation symmetry in spin space, and a VBS, that spontaneously breaks the lattice symmetry, while on the grounds of an LGW-theory, a first order phase transition is generally expected. The quantum Monte Carlo simulations in Ref. [16] show for different dimerization patterns of an $S = 1/2$ antiferromagnetic Heisenberg model on the square lattice that, while most of the dimerization patterns lead to critical exponents consistent with the universality class of the three-dimensional $O(3)$ Heisenberg model, a staggered pattern leads to deviations from it. Hence, the authors raised the possibility of deconfined quantum criticality in this case.

A QPT from a Néel to a paramagnetic phase can be approached from the magnetically ordered side by introducing spin coherent states [18], that lead in general to an $O(3)$ non-linear σ -model [19,20], as in the treatment of the antiferromagnetic quantum Heisenberg model in the context of high temperature superconductivity [21], or, alternatively, employing a CP^1 representation [15]. However, the discussion above, shows that it would be certainly interesting to address the QPT from the VBS side in the case of a dimerized system. When the VBS consists of nearest neighbor dimers, for spins $S = 1/2$, the dimers are naturally described by the possible states of two spins, i.e. by the manifold $SU(2) \otimes SU(2) \simeq SO(4)$. Some time ago, bond-operators were introduced [22–24] for that purpose, that offer an intuitive picture for singlets and triplets. The application of such a representation with different approximation schemes, mostly based on mean-field theory led to rather good descriptions of spin-liquid states in a variety of situations in frustrated [23, 24], dimerized [25,26], and bilayer antiferromagnets [27]. The aim of the present work is to formulate a path integral dealing directly with the $SO(4)$ manifold on the one hand, and with bond-operators on the other hand, enabling a field-theoretic treatment of the transition between dimerized and other possible states.

We consider here two equivalent approaches. The first one deals with the generators of the $SO(4)$ algebra. While previous work [28] used coherent states, we perform the path-integral quantization using the Faddeev–Jackiw symplectic formalism for quantum field-theories with constraints [29,30]. The treatment of constrained systems was initiated by Dirac [31] and continued by Faddeev and Jackiw [29]. These methods were used before for the Heisenberg and t – J model [32–35] showing consistent results with other works where coherent states were used [36]. The formal development is shown in Section 2. The second approach, based on a path-integral

representation of bond-operators, is described in Section 3. In both cases, special emphasis is given to the determination of the measures and constraints appropriate for the respective algebras. We expect in this way to allow for the treatment of fluctuations beyond the mean-field approximation, at the same level as in previous treatments leading to the $O(3)$ non-linear σ -model starting from a Néel configuration. Section 4 illustrates how the obtained path integral representations may be used to reach a field-theory for a spin-Peierls chain. This example was chosen because the effective field-theory is characterized by the presence of a topological term that ensures that in the absence of dimerization, the spin-gap closes. In Appendix A we show explicitly, how to transform from one representation into the other.

2. Path integral formulation for $SO(4)$ fields

2.1. $SO(4)$ operators for a bond

We start by considering the four states $|\mu\rangle$ for a bond joining two $S = 1/2$ states,

$$\begin{aligned} |0\rangle &= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle), \\ |1\rangle &= -\frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle), \\ |2\rangle &= \frac{i}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle), \\ |3\rangle &= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle). \end{aligned} \quad (2.1)$$

We can introduce the Hubbard or X -operators [37] defined as

$$\hat{X}^{\mu\nu} \equiv |\mu\rangle\langle\nu|, \quad (2.2)$$

with $\mu = 0, \dots, 3$. Trivially, they obey the following commutation rules:

$$[\hat{X}^{\mu\nu}, \hat{X}^{\lambda\rho}] = \hat{X}^{\mu\rho}\delta_{\nu\lambda} - \hat{X}^{\lambda\nu}\delta_{\rho\mu} \quad (2.3)$$

and the completeness relation

$$\sum_{\mu} \hat{X}^{\mu\mu} = 1. \quad (2.4)$$

Since we are considering states of $SU(2) \otimes SU(2) \simeq SO(4)$, we have to construct the six generators of $SO(4)$ out of the 16 operators $\hat{X}^{\mu\nu}$. These generators can be written as

$$\begin{aligned} \hat{T}^a &\equiv -i\varepsilon^{abc}\hat{X}^{bc}, \\ \hat{S}^a &\equiv \hat{X}^{0a} + \hat{X}^{a0}, \end{aligned} \quad (2.5)$$

where the Latin indices run over 1, 2, 3. Using the commutation relations (2.3) we obtain

$$\begin{aligned} [\hat{T}^a, \hat{T}^b] &= i\varepsilon^{abc}\hat{T}^c, \\ [\hat{T}^a, \hat{S}^b] &= i\varepsilon^{abc}\hat{S}^c, \\ [\hat{S}^a, \hat{S}^b] &= i\varepsilon^{abc}\hat{T}^c, \end{aligned} \quad (2.6)$$

the commutation relations of the generators of $SO(4)$ [38].

The generators of SU(2) for each site of the bond can be also constructed in the following way:

$$\begin{aligned}\hat{S}_{(1)}^a &= \frac{1}{2}(\hat{T}^a + \hat{S}^a), \\ \hat{S}_{(2)}^a &= \frac{1}{2}(\hat{T}^a - \hat{S}^a),\end{aligned}\quad (2.7)$$

where 1 and 2 denote the two spins making up the bond, such that any spin Hamiltonian can be expressed in terms of the generators of SO(4).

Finally, we consider the Casimir operator in SO(4). The Casimir operator, which commutes with the generators, is given by the sum of the squares of the generators [39] i.e. $\hat{\mathcal{T}}^2 + \hat{\mathcal{S}}^2$. From the relations (2.7), we have $\hat{\mathcal{T}}^2 + \hat{\mathcal{S}}^2 = 1$. There is another bilinear form of operators that commutes with all the generators, namely $\hat{\mathcal{T}} \cdot \hat{\mathcal{S}} = 0$.

2.2. Faddeev–Jackiw theory and path integral for SO(4) fields

In order to develop a path integral representation for quantum system whose operators satisfy general Lie algebras, the coherent-state approach [18] is often used. Here we will instead use the formalism introduced by Faddeev and Jackiw (FJ) [29,30,40], that provides a way to obtain a classical theory consistent with the algebra of the quantum problem without need of dealing with the structure of the corresponding group. In this approach, no formal distinction is made between different forms of constraints like in Dirac’s theory [31], where primary and secondary, first class and second class constraints appear. As shown by Faddeev and Jackiw [29,30,40] constraints can be incorporated iteratively (see also this section and Section 3.2), until the basic brackets for the fields can be determined. Once the classical field-theory is obtained, quantization can proceed via a path integral or in a canonical way.

Our purpose is to construct a classical Lagrangian first order in time derivatives of the SO(4) fields. The terms containing time derivatives will give the corresponding Berry phases. Following FJ, we call these terms canonical. Since the FJ-formalism is not widely used, we will discuss it in some detail, such that the presentation is to a large extent self-contained. Given the Hamiltonian H , that depends on fields y_A , we start by writing a Lagrangian first order in the velocities $\dot{y}_A$,

$$\mathcal{L}(y_A, \dot{y}_A) = \sum_A \dot{y}_A K_A(y_A) - H(y_A). \quad (2.8)$$

Then, the associated Euler–Lagrange equations of motion are (summation over repeated indices is assumed)

$$\left[\frac{\partial K_B}{\partial y_A} - \frac{\partial K_A}{\partial y_B} \right] \dot{y}_B - \frac{\partial H}{\partial y_A} = 0. \quad (2.9)$$

If the matrix defined by

$$M_{AB} \equiv \frac{\partial K_B}{\partial y_A} - \frac{\partial K_A}{\partial y_B} \quad (2.10)$$

is nonsingular, it is possible to write Eq. (2.9) as

$$\dot{y}_B = (M_{AB})^{-1} \frac{\partial H}{\partial y_A}. \quad (2.11)$$

On the other hand, from the Hamiltonian formalism the equations of motion are

$$\dot{y}_B = \{H, y_B\} = \frac{\partial H}{\partial y_A} \{y_A, y_B\}, \quad (2.12)$$

where $\{A, B\}$ denotes the Poisson bracket. Then, comparing (2.11) and (2.12), we see that $(M_{AB})^{-1}$ plays the role of the basic bracket (or generalized bracket) of the Faddeev–Jackiw theory, i.e.

$$\{y_A, y_B\}_{\text{FJ}} = (M_{AB})^{-1}. \quad (2.13)$$

These brackets agree with the Poisson brackets for an unconstrained theory. The generalized bracket between two quantities $F(y_A)$ and $G(y_A)$ is defined by

$$\{F, G\}_{\text{FJ}} = \sum_{AB} \frac{\partial F}{\partial y_A} \{y_A, y_B\}_{\text{FJ}} \frac{\partial G}{\partial y_B}. \quad (2.14)$$

From (2.13) and (2.14) it is straightforward to show that the generalized brackets verify all the properties of the usual Poisson brackets.

In our case, we assume that the first-order Lagrangian can be written in terms of the SO(4)-fields as:

$$\mathcal{L}(\mathcal{T}, \mathcal{S}) = \mathcal{A}_a^T \dot{\mathcal{T}}^a + \mathcal{A}_a^S \dot{\mathcal{S}}^a - V^{(0)}, \quad (2.15)$$

where $\mathcal{A}_a^T$ and $\mathcal{A}_a^S$ are unknown coefficients which must be determined. Since the SO(4)-fields must verify the conditions discussed in Section 2.1, we are in the presence of a constrained theory, where the potential $V^{(0)}$ is

$$V^{(0)} = H + \xi_1 \Omega_1 + \xi_2 \Omega_2, \quad (2.16)$$

with H the proper Hamiltonian, ξ_1 and ξ_2 Lagrange multipliers, and

$$\begin{aligned} \Omega_1 &= \mathcal{T}^2 + \mathcal{S}^2 - 1, \\ \Omega_2 &= \mathcal{T} \cdot \mathcal{S}, \end{aligned} \quad (2.17)$$

are the invariants discussed in Section 2.1, which must be considered here as constraints between the SO(4)-fields.

For the classical Lagrangian (2.15), the set of classical variables in configuration space is $\{y_A\} = \{\mathcal{T}^a, \mathcal{S}^a, \xi_1, \xi_2\}$, the coefficients are $\{K_A\} = \{\mathcal{A}_a^T, \mathcal{A}_a^S\}$, and the corresponding equations of motion are

$$M_{AB} \dot{y}_B = \frac{\partial V^{(0)}}{\partial y_A}. \quad (2.18)$$

After constructing the matrix M_{AB} , it can be readily seen that it is singular because the coefficients K_A are independent of the variables ξ_1, ξ_2 . This can be remedied by promoting the constraints into the canonical terms [40]. For that purpose, we notice first, that when multiplying (2.18) by eigenvectors $v_A^{(i)}$ corresponding to the zero modes, we obtain

$$v_A^{(i)} \frac{\partial V^{(0)}}{\partial y_A} = \frac{\partial V^{(0)}}{\partial \xi_i} = 0, \quad (2.19)$$

putting in evidence, that the zero modes of M_{AB} encode the information of the constraints. For consistency the time evolution of the constraints should also obey

$$\dot{\Omega}_i = 0, \quad i, j = 1, 2. \quad (2.20)$$

These conditions can be incorporated into the Lagrangian with Lagrange multipliers $\lambda_{1,2}$. In this way, discarding total time derivatives, the first iterated Lagrangian results [29,40]

$$\mathcal{L}^{(1)}(\mathcal{T}, \mathcal{S}) = \mathcal{A}_a^T \dot{\mathcal{T}}^a + \mathcal{A}_a^S \dot{\mathcal{S}}^a + \dot{\lambda}_1 \Omega_1 + \dot{\lambda}_2 \Omega_2 - V^{(1)} \quad (2.21)$$

where $V^{(1)} = V^{(0)}|_{\Omega_i=0} = H$. The variables ξ_1, ξ_2 have disappeared because the constraints can now be imposed on the canonical part.

The new set of variables is $y_A = \{\mathcal{T}^a, \mathcal{S}^a, \lambda_1, \lambda_2\}$ and the new 8×8 matrix M_{AB} can be written as

$$M_{AB} = \begin{pmatrix} B^T & \tilde{M} & \tilde{F}_1 \\ -\tilde{M}^T & B^S & \tilde{F}_2 \\ -\tilde{F}_1^T & -\tilde{F}_2^T & 0 \end{pmatrix}, \quad (2.22)$$

where B^T given by

$$B_{ab}^T = \frac{\partial \mathcal{A}_b^T}{\partial \mathcal{T}_a} - \frac{\partial \mathcal{A}_a^T}{\partial \mathcal{T}_b} = \varepsilon_{abc} (\nabla_{\mathcal{T}} \times \mathcal{A}^T)_c, \quad (2.23)$$

and B^S given by

$$B_{ab}^S = \frac{\partial \mathcal{A}_b^S}{\partial \mathcal{S}_a} - \frac{\partial \mathcal{A}_a^S}{\partial \mathcal{S}_b} = \varepsilon_{abc} (\nabla_{\mathcal{S}} \times \mathcal{A}^S)_c, \quad (2.24)$$

are 3×3 antisymmetric matrices. Furthermore, $\tilde{M}$ is a 3×3 matrix given by

$$\tilde{M}_{ab} = \frac{\partial \mathcal{A}_b^S}{\partial \mathcal{T}_a} - \frac{\partial \mathcal{A}_a^T}{\partial \mathcal{S}_b}, \quad (2.25)$$

$\tilde{F}_1$ is a 2×3 matrix given by

$$\tilde{F}_1 = \begin{pmatrix} 2\mathcal{T}_1 & \mathcal{S}_1 \\ 2\mathcal{T}_2 & \mathcal{S}_2 \\ 2\mathcal{T}_3 & \mathcal{S}_3 \end{pmatrix}, \quad (2.26)$$

and $\tilde{F}_2$ is as $\tilde{F}_1$ with $\mathcal{T}$ and $\mathcal{S}$ interchanged.

The unknown coefficients $\mathcal{A}_a^T = \mathcal{A}_a^T(\mathcal{T}, \mathcal{S})$ and $\mathcal{A}_a^S = \mathcal{A}_a^S(\mathcal{T}, \mathcal{S})$ must be determined in such a way that the matrix M_{ab} results nonsingular and the $\text{SO}(4)$ fields verify the following relations

$$\begin{aligned} \{\mathcal{T}^a, \mathcal{T}^b\}_{\text{FJ}} &= -i[\hat{\mathcal{T}}^a, \hat{\mathcal{T}}^b], \\ \{\mathcal{T}^a, \mathcal{S}^b\}_{\text{FJ}} &= -i[\hat{\mathcal{T}}^a, \hat{\mathcal{S}}^b], \\ \{\mathcal{S}^a, \mathcal{S}^b\}_{\text{FJ}} &= -i[\hat{\mathcal{S}}^a, \hat{\mathcal{S}}^b]. \end{aligned} \quad (2.27)$$

These are the classical version of the commutation relations (2.6). From (2.13) and (2.27) we have

$$(M_{AB})^{-1} = \begin{pmatrix} \{\mathcal{T}^a, \mathcal{T}^b\}_{\text{FJ}} & \{\mathcal{T}^a, \mathcal{S}^b\}_{\text{FJ}} & \{\mathcal{T}_a, \lambda_1\}_{\text{FJ}} & \{\mathcal{T}_a, \lambda_2\}_{\text{FJ}} \\ \{\mathcal{S}^a, \mathcal{T}^b\}_{\text{FJ}} & \{\mathcal{S}^a, \mathcal{S}^b\}_{\text{FJ}} & \{\mathcal{S}_a, \lambda_1\}_{\text{FJ}} & \{\mathcal{S}_a, \lambda_2\}_{\text{FJ}} \\ -\{\mathcal{T}_b, \lambda_1\}_{\text{FJ}} & -\{\mathcal{S}_b, \lambda_1\}_{\text{FJ}} & 0 & \{\lambda_1, \lambda_2\}_{\text{FJ}} \\ -\{\mathcal{T}_b, \lambda_1\}_{\text{FJ}} & -\{\mathcal{S}_b, \lambda_1\}_{\text{FJ}} & -\{\lambda_1, \lambda_2\}_{\text{FJ}} & 0 \end{pmatrix}, \quad (2.28)$$

where in (2.28) the elements $\{\mathcal{T}_a, \lambda_i\}_{\text{FJ}}$, $\{\mathcal{S}_a, \lambda_i\}_{\text{FJ}}$ and $\{\lambda_1, \lambda_2\}_{\text{FJ}}$ are unknown but unnecessary. For the determinant of M_{AB} , we obtain:

$$\det M_{AB} = 4D^2, \quad (2.29)$$

where $D = D_1 + D_2$ with

$$D_1 = [\tilde{M}_{ab}(\nabla_S \times \mathcal{A}^S)_b - (\nabla_T \times \mathcal{A}^T)_b \tilde{M}_{ba}](\mathcal{S} \times \mathcal{T})_a, \quad (2.30)$$

and

$$D_2 = [(\nabla_S \times \mathcal{A}^S) \cdot \mathcal{S}][(\nabla_T \times \mathcal{A}^T) \cdot \mathcal{S}] - [(\nabla_S \times \mathcal{A}^S) \cdot \mathcal{T}][(\nabla_T \times \mathcal{A}^T) \cdot \mathcal{T}] + \frac{1}{2}(\mathcal{T}_a \mathcal{T}_d - \mathcal{S}_a \mathcal{S}_d) \varepsilon_{abc} \varepsilon_{def} \tilde{M}_{eb} \tilde{M}_{fc}. \quad (2.31)$$

Imposing the identities (2.27) in (2.28), and after a long but straightforward algebra it is possible to show that the coefficients must satisfy the following set of equations:

$$\begin{aligned} (\nabla_T \times \mathcal{A}^T + \nabla_S \times \mathcal{A}^S) \cdot \mathcal{T} + (\nabla_T \times \mathcal{A}^S + \nabla_S \times \mathcal{A}^T) \cdot \mathcal{S} &= -2, \\ (\nabla_T \times \mathcal{A}^T + \nabla_S \times \mathcal{A}^S) \cdot \mathcal{S} + (\nabla_T \times \mathcal{A}^S + \nabla_S \times \mathcal{A}^T) \cdot \mathcal{T} &= 0, \\ (\nabla_S \times \mathcal{A}^S - \nabla_T \times \mathcal{A}^T) \cdot (\mathcal{T} \times \mathcal{S}) + (\tilde{M}_{ab} + \tilde{M}_{ba})(\mathcal{T}_a \mathcal{T}_b - \mathcal{S}_a \mathcal{S}_b) \\ + \tilde{M}_{aa}(\mathcal{S}^2 - \mathcal{T}^2) + \sum_a \tilde{M}_{aa}(\mathcal{S}_a^2 - \mathcal{T}_a^2) &= 0, \\ D &= -1. \end{aligned} \quad (2.32)$$

A possible solution compatible with the equations above is

$$\nabla_T \times \mathcal{A}^T = \nabla_S \times \mathcal{A}^S, \quad \nabla_S \times \mathcal{A}^T = \nabla_T \times \mathcal{A}^S, \quad \tilde{M}_{ab} = -\tilde{M}_{ba}, \quad (2.33)$$

with

$$\nabla_T \times \mathcal{A}^T = -\mathcal{T}, \quad \nabla_S \times \mathcal{A}^T = -\mathcal{S}, \quad \tilde{M}_{ab} = -\varepsilon_{abc} \mathcal{S}_c, \quad (2.34)$$

as can be easily verified. We notice furthermore that, from the last two equations in (2.34) we have

$$\frac{\partial \mathcal{A}_b^S}{\partial \mathcal{T}_a} = \frac{\partial \mathcal{A}_a^T}{\partial \mathcal{S}_b}. \quad (2.35)$$

The solutions displayed above are, however, not the most general ones. In Appendix A we show explicit forms of $\mathcal{A}^T$ and $\mathcal{A}^S$, that obey Eqs. (2.32) but not all Eqs. (2.34). Nevertheless, it is also shown in Appendix A, that both forms lead to the same Berry phase in the gradient expansion.

Having obtained an effective Lagrangian with a set of coefficients $\mathcal{A}_\alpha^T$, $\mathcal{A}_\alpha^S$ and constraints (2.17) we can write the path integral for the partition function as usual [41]

$$\mathcal{Z} = \int \mathcal{D}\mathcal{T} \mathcal{D}\mathcal{S} \delta(\mathcal{T} \cdot \mathcal{S}) \delta(\mathcal{T}^2 + \mathcal{S}^2 - 1) e^{-S}, \quad (2.36)$$

with the Euclidian action

$$S = \int d\tau \left\{ -i \sum_j (\mathcal{A}_j^T \cdot \partial_\tau \mathcal{T}_j + \mathcal{A}_j^S \cdot \partial_\tau \mathcal{S}_j) + H[\mathcal{T}, \mathcal{S}] \right\}. \quad (2.37)$$

Here we would like to remark a few features. In the measure of the path integral (2.36) only the two constraints enforced by δ -functions appear. No other functional between fields is present because the determinant of the matrix M_{AB} is a constant ($D = -1$). The first term in the action

(2.37), i.e. the Berry phase, depends on the coefficients $\mathcal{A}^T$ and $\mathcal{A}^S$, that have to fulfill (2.32). Hence, they are defined up to a gauge transformation,

$$\mathcal{A}_a^T \rightarrow \mathcal{A}_a^T + \frac{\partial \Lambda}{\partial T_a}, \quad \mathcal{A}_a^S \rightarrow \mathcal{A}_a^S + \frac{\partial \Lambda}{\partial S_a}, \quad (2.38)$$

with $\Lambda = \Lambda(\mathcal{A}^T, \mathcal{A}^S)$ a scalar function, in a similar way as in the SU(2) case. In this way, we have obtained a path integral for the SO(4) fields that is fully consistent with the algebra of the quantum problem.

3. Bond-fields formulation of bond variables

3.1. Bond-fields for spin-states on a bond

It is usual for constrained systems, where it is necessary to deal with operators that do not satisfy canonical commutation rules, to introduce slave particles by decoupling the original operators [42]. In the frame of the Hubbard operators $X^{\mu\nu}$ defined in (2.2), the following decoupling can be used,

$$X^{ab} = t_a^\dagger t_b, \quad X^{0a} = s^\dagger t_a, \quad (3.1)$$

with $a, b = 1, 2, 3$, and where $\{t_a, t_a^\dagger, s, s^\dagger\}$ satisfy bosonic commutation rules

$$[t_a, t_b^\dagger] = \delta_{ab}, \quad [s, s^\dagger] = 1, \quad [s^\dagger, t_a] = 0. \quad (3.2)$$

Using (3.1) it is easy to show that the commutation rules (2.3) are satisfied. In addition, the completeness condition (2.4) can be written as

$$s^\dagger s + t_a^\dagger t_a = 1. \quad (3.3)$$

From Eqs. (2.5), (2.7) and (3.1) we obtain

$$\begin{aligned} S_{(1)}^a &= \frac{1}{2}(s^\dagger t_a + t_a^\dagger s - i\varepsilon_{abc} t_b^\dagger t_c), \\ S_{(2)}^a &= \frac{1}{2}(-s^\dagger t_a - t_a^\dagger s - i\varepsilon_{abc} t_b^\dagger t_c), \end{aligned} \quad (3.4)$$

that exactly correspond to the relation between spin- and bond-operators introduced by Sachdev and Bhatt [23].

As the path integral (2.36) shows, only four real variables are independent. Therefore, on passing from bond-operators to bond-fields, four constraints are needed. One of them is the completeness condition

$$\varphi_1 \equiv s^* s + t_a^* t_a - 1 = 0. \quad (3.5)$$

In order to obtain the remaining conditions, we use the well-known CP¹ representation [42] for the spin-fields $S_{(1)}$ and $S_{(2)}$,

$$S_{(1)}^a = \frac{1}{2} \bar{z} \sigma^a z, \quad S_{(2)}^a = \frac{1}{2} \bar{\omega} \sigma^a \omega, \quad (3.6)$$

where σ^a are the Pauli matrices. The CP¹ fields, $\bar{z} = (z_1^*, z_2^*)$ and $\bar{\omega} = (\omega_1^*, \omega_2^*)$, fulfill the conditions

$$\bar{z}z = 1, \quad \bar{\omega}\omega = 1. \quad (3.7)$$

On the basis of Eqs. (3.4) and (3.6), the following relations between bond-fields and CP^1 variables can be obtained:

$$\begin{aligned} s &= \frac{1}{\sqrt{2}}(z_1\omega_2 - z_2\omega_1), \\ t_1 &= \frac{1}{\sqrt{2}}(z_2\omega_2 - z_1\omega_1), \\ t_2 &= -\frac{i}{\sqrt{2}}(z_1\omega_1 + z_2\omega_2), \\ t_3 &= \frac{1}{\sqrt{2}}(z_1\omega_2 + z_2\omega_1). \end{aligned} \quad (3.8)$$

These equations lead to two additional constraints for the bond-fields:

$$\begin{aligned} \varphi_2 &\equiv ss - t_a t_a = 0, \\ \varphi_3 &\equiv s^* s^* - t_a^* t_a^* = 0. \end{aligned} \quad (3.9)$$

As can be seen from (3.4), the theory defined in terms of the bond-fields contains a gauge degree of freedom such that, the remaining constraint will appear as a gauge-fixing condition, that we discuss in the next section.

3.2. Faddeev–Jackiw theory and path integral formulation for bond-operators

In this section we will develop the FJ-formalism for bond-operators. The procedure will parallel that of Section 2.2, but due to a gauge freedom, it will be iterated, until the condition for gauge fixing is incorporated in the theory.

Our starting point is the classical Lagrangian

$$\mathcal{L} = -\frac{i}{2}(s^* \dot{s} - s \dot{s}^* + t_a^* \dot{t}_a - t_a \dot{t}_a^*) - V^{(0)}, \quad (3.10)$$

where $V^{(0)} = H(s^*, s, t_a^*, t_a) + \xi_i \varphi_i$, $H(s^*, s, t_a^*, t_a)$ is the spin Hamiltonian written in terms of the bond-fields, ξ_i are Lagrange multipliers and the constraints φ_i with $i = 1, 2, 3$ were defined in Eqs. (3.5) and (3.9) in the last subsection. As in previous bond-operator treatments [23], we have adopted the usual kinetic Lagrangian for bosons. As we will see below, this is consistent with the $\text{SO}(4)$ algebra.

From the Lagrangian (3.10), the set of classical variables is $\{y_A\} = \{q_\alpha, \xi_i\}$, where $q_\alpha = \{s, s^*, t_a, t_a^*\}$, with the index $\alpha = 1, \dots, 8$. The corresponding matrix M_{AB} is singular, because the coefficients K_A do not contain the variables ξ_i . In this case the matrix M_{AB} has three zero eigenvectors $v^{(i)}$. Multiplying the Euler–Lagrange equations (2.18) by $v^{(i)}$, we obtain as in Section 2.2

$$v_A^{(i)} \frac{\partial V^{(0)}}{\partial y_A} = \frac{\partial V^{(0)}}{\partial \xi_i} = 0, \quad (3.11)$$

that leads to $\varphi_i = 0$. As described in Section 2.2 and in Refs. [29,40] we incorporate the constraints (3.11) into the kinetic part of the Lagrangian using new Lagrange multipliers λ_i . The first iterated Lagrangian results

$$\mathcal{L}^{(1)}(\mathcal{T}, \mathcal{S}) = -\frac{i}{2}(\dot{s}^* s - \dot{s} s^* + \dot{t}_a^* t_a - \dot{t}_a t_a^*) + \dot{\lambda}_i \varphi_i - V^{(1)}, \quad (3.12)$$

where $V^{(1)} = V^{(0)}|_{\varphi_i=0} = H$. For the Lagrangian (3.12) the new set of variables is $y_A = \{q_\alpha, \lambda_i\}$ and the new matrix M_{AB} is

$$M_{AB} = \begin{bmatrix} f_{\alpha\beta} & \frac{\partial \varphi_i}{\partial q_\alpha} \\ -(\frac{\partial \varphi_i}{\partial q_\beta})^T & 0 \end{bmatrix}, \quad (3.13)$$

where

$$f_{\alpha\beta} = \begin{pmatrix} 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \\ 0 & 0 & 0 & i\delta_{ab} \\ 0 & 0 & -i\delta_{ab} & 0 \end{pmatrix}. \quad (3.14)$$

Note that $f_{\alpha\beta}^{-1}$ is the matrix formed by the classical extension of the commutations relations for bond fields.

As the matrix M_{AB} is antisymmetric with an odd number of rows and columns (11×11), it is singular. After the first iteration, M_{AB} has only one zero-eigenvector $\mathbf{u}$ [43]

$$\mathbf{u}^T = \left(-\frac{\partial \varphi_1}{\partial q_\alpha} f_{\alpha\beta}^{-1}, 1, 0, 0 \right) = (-is, is^*, -it_a, it_a^*, 1, 0, 0). \quad (3.15)$$

As before, the new constraint is obtained multiplying the Euler–Lagrange equation (2.18) by the zero-eigenvector $\mathbf{u}$, i.e. the new constraint is

$$0 = u_A^T \frac{\partial V^{(1)}}{\partial y_A} = -\frac{\partial \varphi_1}{\partial q_\alpha} f_{\alpha\beta}^{-1} \frac{\partial V^{(1)}}{\partial q_\beta} = \{\varphi_1, V^{(1)}\} = \dot{\varphi}_1, \quad (3.16)$$

where we have used Eqs. (3.15) and (2.14). Therefore, no new constraint arises from Eq. (3.16) because φ_1 is already a constraint and its time evolution is also a constraint for consistency. This fact is related to the existence of a gauge degree of freedom associated with the completeness condition φ_1 .

In order to obtain a gauge fixing condition φ_4 as a new constraint, we will repeat the process introducing a new Lagrangian $\mathcal{L}^{(2)}$

$$\mathcal{L}^{(2)}(\mathcal{T}, \mathcal{S}) = -\frac{i}{2}(\dot{s}^* s - \dot{s} s^* + \dot{t}_a^* t_a - \dot{t}_a t_a^*) + \dot{\lambda}_i \varphi_i + \dot{\lambda}_4 \varphi_4 - V^{(2)}, \quad (3.17)$$

where $V^{(2)} = V^{(1)}|_{\varphi_i=0} = H$ and the set of variables of the new configuration space is $\{y_A\} = \{q_\alpha, \lambda_i, \lambda_4\}$. We will choose a gauge fixing condition φ_4 in such a way that the new matrix M_{AB} is nonsingular. In other words

$$\det[M_{AB}] = 16 \left[\frac{\partial \varphi_4}{\partial s} s - \frac{\partial \varphi_4}{\partial s^*} s^* + \frac{\partial \varphi_4}{\partial t_a} t_a - \frac{\partial \varphi_4}{\partial t_a^*} t_a^* \right]^2 = 16\Lambda^2 \quad (3.18)$$

must be different from zero. Computing the inverse of M_{AB} , we obtain the following FJ brackets between bond fields:

$$\begin{aligned} \{s, s\}_{\text{FJ}} &= \{s^*, s^*\}_{\text{FJ}} = 0, \\ \{s, s^*\}_{\text{FJ}} &= i(1 - ss^*) + (sw_1^* - s^*w_1), \\ \{s, t_a\}_{\text{FJ}} &= t_a w_1 - s v_a, \end{aligned}$$

$$\begin{aligned}
\{s, t_a^*\}_{\text{FJ}} &= i s^* t_a + (s v_a^* - t_a^* w_1), \\
\{s^*, t_a\}_{\text{FJ}} &= -i s t_a^* + (s^* v_a - t_a w_1^*), \\
\{s^*, t_a^*\}_{\text{FJ}} &= t_a^* w_1^* - s^* v_a^*, \\
\{t_a, t_b\}_{\text{FJ}} &= -(t_a v_b - t_b v_a), \\
\{t_a, t_b^*\}_{\text{FJ}} &= i(\delta_{ab} - t_a^* t_b) + (t_a v_b^* - t_b^* v_a), \\
\{t_a^*, t_b^*\}_{\text{FJ}} &= -(t_a^* v_b^* - t_b^* v_a^*),
\end{aligned} \tag{3.19}$$

where

$$\begin{aligned}
w_1 &= -\frac{i}{\Lambda} \left[(1 - s^* s) \frac{\partial \varphi_4}{\partial s^*} + s^* \frac{\partial \varphi_4}{\partial t_a^*} t_a \right], \\
v_a &= -\frac{i}{\Lambda} \left[(\delta_{ab} - t_a^* t_b) \frac{\partial \varphi_4}{\partial t_b^*} + \frac{\partial \varphi_4}{\partial s^*} s t_a^* \right],
\end{aligned} \tag{3.20}$$

and $a = 1, 2, 3$. Note that on taking into account the constraints, the FJ brackets are different from the usual bosonic commutation rules. As expected, using (3.19), for any explicit form of a gauge fixing, the SO(4) algebra is fulfilled.

Finally, the partition function for the bond-fields can be written as [41]

$$\mathcal{Z} = \int \mathcal{D}s^* \mathcal{D}s \mathcal{D}t_a^* \mathcal{D}t_a (\det[M_{AB}])^{1/2} \delta[\varphi_4] \delta[\varphi_1] \delta[\varphi_2] \delta[\varphi_3] e^{-S}, \tag{3.21}$$

where

$$S = \int d\tau [(s^* \dot{s} + t_a^* \dot{t}_a) + H], \tag{3.22}$$

and $(\det[M_{AB}])^{1/2} = 4\Lambda$ is equivalent to the Faddeev–Popov (FP) determinant Δ_{FP} in gauge theories [41].

Before closing this section, we would like to remark that bond-operators were frequently used at the mean field level, or closely related approximations, where the full form of (3.21) is not respected [23–27]. There, only the effective Lagrangian L and φ_1 are considered while $\varphi_2, \varphi_3, \varphi_4$ and $\Delta_{\text{FP}} = (\det[M_{AB}])^{1/2}$ are missing. While on a mean-field level the measure and constraints are not crucial, their presence is important when considering the effect of fluctuations. We show in Section 4.2.3 how, dealing with them, leads to the correct long-wavelength effective action.

We will show in the following with the one-dimensional spin-Peierls systems as an example, how the corresponding continuum theory can be recovered starting with a path integral for the dimerized state.

4. Spin-Peierls chain

As an application of the formulations developed above, we consider a spin-Peierls chain. On the one hand, this is a well-known system. On the other hand, the corresponding field-theory has a topological term, closely related to the one present in the field-theory for the antiferromagnetic Heisenberg model. In order to obtain it, a proper treatment of the fluctuations is needed.

The spin-Peierls Hamiltonian in one dimension can be written as

$$H_{\text{SP}} = J \sum_i [1 + (-1)^i \Delta] \mathbf{S}_i \cdot \mathbf{S}_{i+1}, \tag{4.1}$$

where $\Delta < 1$ indicates the degree of dimerization. For $\Delta = 1$, the system breaks down into a set of decoupled dimers, while for $\Delta = 0$, it reduces to the antiferromagnetic Heisenberg chain.

We can introduce strong bonds given by $(i, i + 1)$ with $i = 2j$, $j \in \mathbb{Z}$. Using this notation the spin-Peierls Hamiltonian (4.1) reads

$$H_{\text{SP}} = J \sum_j [(1 + \Delta) \mathbf{S}_{j,(1)} \cdot \mathbf{S}_{j,(2)} + (1 - \Delta) \mathbf{S}_{j,(2)} \cdot \mathbf{S}_{j+1,(1)}], \quad (4.2)$$

where the dimerization pattern is described by bonds labeled by the index j .

4.1. Continuum limit with $\text{SO}(4)$ fields

Close to the point where the system goes over to the state appropriate for the antiferromagnetic Heisenberg chain, a large correlation length should be expected, such that the continuum limit is appropriate. Using (2.7), H_{SP} can be written in terms of the $\text{SO}(4)$ -fields as follows

$$H_{\text{SP}} = \frac{J}{4} \sum_j [(1 + \Delta)(\mathcal{T}_j^2 - \mathcal{S}_j^2) + (1 - \Delta)(\mathcal{T}_j - \mathcal{S}_j) \cdot (\mathcal{T}_{j+1} + \mathcal{S}_{j+1})]. \quad (4.3)$$

According to (2.36), the path-integral for this Hamiltonian is given by

$$Z = \int \mathcal{D}\mathcal{T} \mathcal{D}\mathcal{S} \delta(\mathcal{T} \cdot \mathcal{S}) \delta(\mathcal{T}^2 + \mathcal{S}^2 - 1) e^{-S}, \quad (4.4)$$

with the action in imaginary time

$$S = \int d\tau \left\{ -i \sum_j (\mathcal{A}_j^{\mathcal{T}} \cdot \partial_\tau \mathcal{T}_j + \mathcal{A}_j^{\mathcal{S}} \cdot \partial_\tau \mathcal{S}_j) + H_{\text{SP}}[\mathcal{T}, \mathcal{S}] \right\}. \quad (4.5)$$

We approach the continuum limit by performing a gradient expansion around a configuration that is appropriate for large Δ , where the Hamiltonian is dominated by

$$H_\Delta = \frac{J}{4} \sum_j (1 + \Delta)(\mathcal{T}_j^2 - \mathcal{S}_j^2). \quad (4.6)$$

From a mean-field point of view, the lowest energy is obtained by maximizing $\mathcal{S}^2$ and consequently minimizing $\mathcal{T}^2$. The classical configuration of lowest energy is given by $\mathcal{S}^2 = 1$, so that we take

$$\mathcal{S}_j = C_j \mathbf{n}_j \quad (4.7)$$

with $\mathbf{n}_j^2 = 1$, such that the condition $\mathcal{T}_j^2 + \mathcal{S}_j^2 = 1$ leads to

$$C_j = \sqrt{1 - \mathcal{T}_j^2}. \quad (4.8)$$

Since $\mathcal{T}_j$ is proportional to the change of $\mathcal{S}_j$, i.e.

$$\mathcal{T}_j \sim \partial_\mu \mathcal{S}_j, \quad (4.9)$$

the fields entering the action are

$$\begin{aligned} \mathcal{S}_j &= \mathbf{n}_j \sqrt{1 - a^2 \ell_j^2}, \\ \mathcal{T}_j &= a \ell_j, \end{aligned} \quad (4.10)$$

where a is the lattice constant of the new lattice. In addition, $\ell \cdot \mathbf{n} = 0$.

After defining the fields for the gradient expansion, we consider the different pieces of the action. First we have

$$\mathcal{T}_j^2 - \mathcal{S}_j^2 = 2a^2 \ell_j^2 - 1. \quad (4.11)$$

Hence, the modes described by the field ℓ_j are massive. Since we are in $1 + 1$ dimensions, we perform the gradient expansion up to $\mathcal{O}(a^2)$. For the rest of the terms coming from the Hamiltonian we have,

$$\begin{aligned} \mathcal{T}_j \cdot \mathcal{T}_{j+1} &\simeq a^2 \ell_j^2, \\ \mathcal{T}_j \cdot \mathcal{S}_{j+1} &\simeq a^2 \ell_j \cdot \partial_x \mathbf{n}_j, \\ \mathcal{S}_j \cdot \mathcal{T}_{j+1} &\simeq a^2 \mathbf{n}_j \cdot \partial_x \ell_j, \\ \mathcal{S}_j \cdot \mathcal{S}_{j+1} &\simeq 1 - a^2 \ell_j^2 + \frac{1}{2} a^2 \mathbf{n}_j \cdot \partial_x^2 \mathbf{n}_j. \end{aligned} \quad (4.12)$$

Putting all the contributions together, and going over to the continuum, we have

$$H_{\text{SP}}[\mathcal{T}, \mathcal{S}] \rightarrow Ja \int dx \left\{ \ell^2 + (1 - \Delta) \left[\frac{1}{2} \ell \cdot \partial_x \mathbf{n} + \frac{1}{8} (\partial_x \mathbf{n})^2 \right] \right\}. \quad (4.13)$$

Next we deal with the Berry phase. Here we have

$$S_B = -i \int d\tau \sum_j (\mathcal{A}_j^{\mathcal{T}} \cdot \partial_\tau \mathcal{T}_j + \mathcal{A}_j^{\mathcal{S}} \cdot \partial_\tau \mathcal{S}_j). \quad (4.14)$$

Since from the discussion above, the $\text{SO}(4)$ -fields have only a smooth spatial dependence, we can concentrate on one site. Furthermore, since from (4.10) $|\mathcal{T}| \sim a$, we can expand the vector potentials accordingly. In lowest order we have from (2.34),

$$\nabla_{\mathcal{T}} \times \mathcal{A}^{\mathcal{T}}|_{\mathcal{T}=0} = \nabla_{\mathcal{S}} \times \mathcal{A}^{\mathcal{S}}|_{\mathcal{T}=0} = 0. \quad (4.15)$$

Hence, we can write

$$\begin{aligned} \mathcal{A}_a^{\mathcal{T}}(\mathcal{T}=0, \mathcal{S}) &= \frac{\partial}{\partial T^a} \phi^{\mathcal{T}}(\mathcal{T}, \mathcal{S}), \\ \mathcal{A}_a^{\mathcal{S}}(\mathcal{T}=0, \mathcal{S}) &= \frac{\partial}{\partial S^a} \phi^{\mathcal{S}}(\mathcal{T}, \mathcal{S}), \end{aligned} \quad (4.16)$$

where $\phi^{\mathcal{T}}$ and $\phi^{\mathcal{S}}$ are scalar functions. Such terms can be gauged away when necessary.

The expansion of the fields $\mathcal{A}^{\mathcal{T}}$ and $\mathcal{A}^{\mathcal{S}}$ in powers of T^a leads to

$$\begin{aligned} \mathcal{A}_a^{\mathcal{T}}(\mathcal{T}, \mathcal{S}) &= \mathcal{A}_a^{\mathcal{T}}(\mathcal{T}=0, \mathcal{S}) + \frac{\partial \mathcal{A}_a^{\mathcal{T}}}{\partial T^b} \Big|_{\mathcal{T}=0} T^b + \mathcal{O}(a^2), \\ \mathcal{A}_a^{\mathcal{S}}(\mathcal{T}, \mathcal{S}) &= \mathcal{A}_a^{\mathcal{S}}(\mathcal{T}=0, \mathcal{S}) + \frac{\partial \mathcal{A}_a^{\mathcal{S}}}{\partial T^b} \Big|_{\mathcal{T}=0} T^b + \mathcal{O}(a^2), \end{aligned} \quad (4.17)$$

where due to the presence of one time derivative in the Berry phase, we need to consider only terms up to $\mathcal{O}(a)$. Introducing the expansion into (4.14) leads to

$$\begin{aligned} \mathcal{A}^{\mathcal{T}} \cdot \partial_\tau \mathcal{T} + \mathcal{A}^{\mathcal{S}} \cdot \partial_\tau \mathcal{S} &= \mathcal{A}^{\mathcal{T}}(0, \mathcal{S}) \cdot \partial_\tau \mathcal{T} + \frac{\partial \mathcal{A}_a^{\mathcal{T}}}{\partial T^b} \Big|_{\mathcal{T}=0} T^b \partial_\tau T^a \\ &\quad + \mathcal{A}^{\mathcal{S}}(0, \mathcal{S}) \cdot \partial_\tau \mathcal{S} + \frac{\partial \mathcal{A}_a^{\mathcal{S}}}{\partial T^b} \Big|_{\mathcal{T}=0} T^b \partial_\tau S^a. \end{aligned} \quad (4.18)$$

From (2.34) we have

$$\begin{aligned}\frac{\partial \mathcal{A}_a^T}{\partial T^b} &= \frac{\partial \mathcal{A}_b^T}{\partial T^a} + \varepsilon^{abc} T^c, \\ \frac{\partial \mathcal{A}_a^S}{\partial T^b} &= \frac{\partial \mathcal{A}_b^S}{\partial T^a} + \varepsilon^{abc} S^c,\end{aligned}\quad (4.19)$$

such that using (2.35), we arrive at

$$\begin{aligned}\mathcal{A}^T \cdot \partial_\tau \mathbf{T} + \mathcal{A}^S \cdot \partial_\tau \mathbf{S} &= \partial_\tau (\mathcal{A}^T \cdot \mathbf{T}) + \mathcal{A}^S(0, \mathbf{S}) \cdot \partial_\tau \mathbf{S} + \varepsilon^{abc} \partial_\tau S^a T^b S^c \\ &= \varepsilon^{abc} \partial_\tau S^a T^b S^c,\end{aligned}\quad (4.20)$$

where the first term can be discarded since it is a total time derivative and the second one can be gauged away, as discussed after Eq. (4.16). Inserting the relations (4.10), we finally have for the Berry phase in the continuum limit,

$$S_B = - \int d\tau dx \, \boldsymbol{\ell} \cdot (\mathbf{n} \times \partial_\tau \mathbf{n}). \quad (4.21)$$

Going back to (4.5), we have for the action after the gradient expansion,

$$\begin{aligned}S &= -i \int d\tau dx \, \boldsymbol{\ell} \cdot (\mathbf{n} \times \partial_\tau \mathbf{n}) \\ &\quad + Ja \int d\tau dx \left\{ \ell^2 + (1 - \Delta) \left[\frac{1}{2} \boldsymbol{\ell} \cdot \partial_x \mathbf{n} + \frac{1}{8} (\partial_x \mathbf{n})^2 \right] \right\}.\end{aligned}\quad (4.22)$$

At this point $\boldsymbol{\ell}$ can be integrated out. Since the action is quadratic in this field, we can simply consider the saddle point for $\boldsymbol{\ell}$, that leads to

$$\ell^a = \frac{1}{2Ja} \left[i \varepsilon^{abc} n^b \partial_\tau n^c - \frac{Ja}{2} (1 - \Delta) \partial_x n^a \right]. \quad (4.23)$$

Inserting this into the action, we finally obtain

$$\begin{aligned}S &= \int d\tau dx \left[\frac{1}{4Ja} (\partial_\tau \mathbf{n})^2 + \frac{Ja}{16} (1 - \Delta^2) (\partial_x \mathbf{n})^2 \right] \\ &\quad + i \frac{(1 - \Delta)}{4} \int d\tau dx \, \mathbf{n} \cdot (\partial_\tau \mathbf{n} \times \partial_x \mathbf{n}).\end{aligned}\quad (4.24)$$

The coupling constant and spin-wave velocity are given by

$$g = \frac{4}{(1 - \Delta^2)^{1/2}}, \quad (4.25)$$

and

$$c = \frac{J}{2} [1 - \Delta^2]^{1/2}. \quad (4.26)$$

The same result can be achieved performing the same treatment as for the Heisenberg model [42].

The action (4.24) corresponds to an O(3) non-linear σ -model with a topological term $i\theta Q$, with $\theta = S(1 - \Delta)/2$, for $S = 1/2$, and Q given by the integral in the last term of (4.24), acquiring values $4n\pi$, with n an integer. For the antiferromagnetic Heisenberg chain ($\Delta = 0$), it is

responsible for the absence of a gap for half-integer S , while a gap is present for S integer, as first discussed by Haldane [44,45] some time ago. Affleck and Haldane [46–48] related the $O(3)$ non-linear σ -model with a topological term to the Wess–Zumino–Witten non-linear σ -model with topological coupling constant $k = 1$, a conformal field theory that constitutes an attractive fixed point for antiferromagnetic Heisenberg chains with half-integer spin. Based on the conformal field-theory, the critical behavior for $\Delta \neq 0$ was discussed by Affleck et al. [49], showing that the mass gap opens as $m \propto \Delta^{2/3}/|\ln \Delta|^{1/2}$. Numerical simulations with a cluster algorithm [50] confirmed later the correctness of the identification of the action (4.24) with the WZW conformal field theory, and showed that for $\Delta \neq 0$, a gap opens. Hence, our path integral formulation allowed us to start from a dimerized phase and take into account the relevant long-wavelength fluctuations that describe the critical behavior of the system in the limit $\Delta \rightarrow 0$.

4.2. Continuum limit with bond-fields

As a first step, we have to identify as in the previous discussion, slow and fast components of the bond-fields, in order to allow for a gradient expansion. For that purpose, we use a staggered CP^1 representation, that was previously introduced for the t – J model [35]. We discuss it shortly here, in order to allow for a self-contained presentation.

4.2.1. Staggered CP^1 representation

We consider now the fact that the spin-fields $S_{(1)}$ and $S_{(2)}$ on a bond are staggered with respect to each other, and introduce a CP^1 representation, such that

$$\begin{aligned} S_{(1)}^a &= \bar{z}^{(1)} \sigma^a z^{(1)}, \\ S_{(2)}^a &= z_{\alpha}^{(2)} \sigma_{\alpha\beta}^y \sigma_{\beta\gamma}^a \sigma_{\gamma\delta}^y \bar{z}_{\delta}^{(2)*}, \end{aligned} \quad (4.27)$$

where $\bar{z}^{(i)} z^{(i)} = 1$, $i = 1, 2$. On the other hand, making the following replacements

$$\begin{aligned} z_1 &\rightarrow z_1^{(1)}, & z_2 &\rightarrow z_2^{(1)}, \\ \omega_1 &\rightarrow -i z_2^{(2)*}, & \omega_2 &\rightarrow i z_1^{(2)*}, \end{aligned} \quad (4.28)$$

in the expressions (3.8), the bond-fields can be written as follows:

$$\begin{aligned} s &= i \frac{\sqrt{2}}{2} \bar{z}^{(2)} z^{(1)}, \\ t_a &= i \frac{\sqrt{2}}{2} \bar{z}^{(2)} \sigma^a z^{(1)}. \end{aligned} \quad (4.29)$$

From the relations above it is easy to show that the completeness relation

$$s^* s + t_a^* t_a = z_{\alpha}^{(1)*} z_{\alpha}^{(1)} z_{\beta}^{(2)*} z_{\beta}^{(2)} = 1, \quad (4.30)$$

and that the constraints

$$s s - t_a t_a = s^* s^* - t_a^* t_a^* = 0 \quad (4.31)$$

also hold.

The Berry phase is given by

$$s^* \dot{s} + t_a^* \dot{t}_a = \bar{z}^{(1)} \partial_{\tau} z^{(1)} - \bar{z}^{(2)} \partial_{\tau} z^{(2)}. \quad (4.32)$$

This is the form of the Berry phase in the staggered CP^1 representation [35].

4.2.2. Slow and fast components of the bond-fields

For each bond we can define new fields

$$\begin{aligned}\tilde{z} &= \frac{1}{2}[z^{(1)} + z^{(2)}], \\ a\zeta &= \frac{1}{2}[z^{(2)} - z^{(1)}].\end{aligned}\quad (4.33)$$

Due to the constraints satisfied by the fields $z^{(i)}$, we have

$$\begin{aligned}(\bar{\tilde{z}} + a\bar{\zeta})(\tilde{z} + a\zeta) &= 1, \\ (\bar{\tilde{z}} - a\bar{\zeta})(\tilde{z} - a\zeta) &= 1,\end{aligned}\quad (4.34)$$

leading to constraints for the fields $\tilde{z}$ and ζ ,

$$\bar{\tilde{z}}\zeta + \bar{\zeta}\tilde{z} = 0, \quad (4.35)$$

$$\bar{\tilde{z}}\tilde{z} + a^2\bar{\zeta}\zeta = 1. \quad (4.36)$$

We then introduce new fields

$$\tilde{z} = z\sqrt{1 - a^2\bar{\zeta}\zeta}, \quad (4.37)$$

such that the constraint (4.36) goes over into

$$\bar{\tilde{z}}z = 1, \quad (4.38)$$

and the constraint (4.35) translates into

$$\bar{\tilde{z}}\zeta + \bar{\zeta}z = 0. \quad (4.39)$$

The fields z and ζ defined above correspond to smooth configurations.

Next, we can express the bond-fields in terms of the fields z and ζ as follows:

$$\begin{aligned}s &= i\frac{\sqrt{2}}{2}[1 + a(\bar{\zeta}z - \bar{\tilde{z}}\zeta) - 2a^2\bar{\zeta}\zeta], \\ t_a &= i\frac{\sqrt{2}}{2}[\bar{\tilde{z}}\sigma^a z(1 - a^2\bar{\zeta}\zeta) + a(\bar{\zeta}\sigma^a z - \bar{\tilde{z}}\sigma^a \zeta) - a^2\bar{\zeta}\sigma^a \zeta],\end{aligned}\quad (4.40)$$

where we keep contributions up to $\mathcal{O}(a^2)$. Guided by the expression of t_a , we define the following vectors,

$$\begin{aligned}\boldsymbol{\Omega} &= \bar{\tilde{z}}\boldsymbol{\sigma}z, \\ \boldsymbol{L} &= \bar{\tilde{z}}\boldsymbol{\sigma}\zeta, \\ \boldsymbol{L}^\dagger &= \bar{\zeta}\boldsymbol{\sigma}z, \\ \boldsymbol{m} &= \bar{\zeta}\boldsymbol{\sigma}\zeta.\end{aligned}\quad (4.41)$$

For later convenience, we define the following two vectors in addition to $\boldsymbol{\Omega}$ and $\boldsymbol{m}$,

$$\boldsymbol{L}_R \equiv \frac{1}{2}(\boldsymbol{L} + \boldsymbol{L}^\dagger) = \frac{1}{2}(\bar{\tilde{z}}\boldsymbol{\sigma}\zeta + \bar{\zeta}\boldsymbol{\sigma}z), \quad (4.42)$$

$$\boldsymbol{L}_I \equiv -\frac{i}{2}(\boldsymbol{L} - \boldsymbol{L}^\dagger) = -\frac{i}{2}(\bar{\tilde{z}}\boldsymbol{\sigma}\zeta - \bar{\zeta}\boldsymbol{\sigma}z). \quad (4.43)$$

Further relations can be obtained by using that

$$\boldsymbol{\Omega} \cdot \mathbf{L} = \bar{z}\zeta, \quad \boldsymbol{\Omega} \cdot \mathbf{L}^\dagger = \bar{\zeta}z, \quad (4.44)$$

such that

$$\bar{\zeta}z - \bar{z}\zeta = \boldsymbol{\Omega} \cdot (\mathbf{L}^\dagger - \mathbf{L}) = -2i\boldsymbol{\Omega} \cdot \mathbf{L}_I. \quad (4.45)$$

Using the constraint (4.39) it can be also shown that

$$\mathbf{L}_I^2 = \bar{\zeta}\zeta. \quad (4.46)$$

With the relations above, we can rewrite (4.40) as follows

$$\begin{aligned} s &= \frac{i}{\sqrt{2}} [1 - 2ia\boldsymbol{\Omega} \cdot \mathbf{L}_I - 2a^2(\mathbf{L}_I)^2], \\ t_a &= \frac{i}{\sqrt{2}} [\Omega_a - 2iaL_{Ia} - a^2(\mathbf{L}_I^2\Omega_a + m_a)]. \end{aligned} \quad (4.47)$$

Due to the constraints (4.38) and (4.39), the vector-fields fulfill the following conditions:

$$\begin{aligned} \boldsymbol{\Omega}^2 &= 1, \\ \boldsymbol{\Omega} \cdot \mathbf{L}_R &= 0, \\ \mathbf{L}_I \cdot \mathbf{L}_R &= 0, \\ \mathbf{m} \cdot \mathbf{L}_R &= 0. \end{aligned} \quad (4.48)$$

There we can see that the vector-fields $\boldsymbol{\Omega}$, $\mathbf{L}_I$, and $\mathbf{m}$ are coplanar, so that they can be described as linear combinations of two orthogonal fields in that plane. We choose them to be $\boldsymbol{\Omega}$ and $\boldsymbol{\Omega} \times \mathbf{L}_R$. Using the form of $\boldsymbol{\Omega} \times \mathbf{L}_R$ expressed in terms of the fields z and ζ (Eq. (4.41) and Eq. (4.42)) we can write

$$\mathbf{L}_I = (\boldsymbol{\Omega} \cdot \mathbf{L}_I)\boldsymbol{\Omega} - (\boldsymbol{\Omega} \times \mathbf{L}_R), \quad (4.49)$$

and

$$\mathbf{m} = [2(\boldsymbol{\Omega} \cdot \mathbf{L}_I)^2 - \mathbf{L}_I^2]\boldsymbol{\Omega} - 2(\boldsymbol{\Omega} \cdot \mathbf{L}_I)(\boldsymbol{\Omega} \times \mathbf{L}_R). \quad (4.50)$$

Inserting the expressions for $\mathbf{L}_I$ and $\mathbf{m}$ into (4.47), we have

$$\begin{aligned} s &= \frac{i}{\sqrt{2}} [1 - 2ia\varphi - 2a^2(\varphi^2 + \mathbf{L}_R^2)], \\ t &= \frac{i}{\sqrt{2}} \{ \boldsymbol{\Omega} - 2ia[\varphi\boldsymbol{\Omega} - (\boldsymbol{\Omega} \times \mathbf{L}_R)] - 2a^2\varphi[\varphi\boldsymbol{\Omega} - (\boldsymbol{\Omega} \times \mathbf{L}_R)] \}, \end{aligned} \quad (4.51)$$

where we introduced $\varphi \equiv \boldsymbol{\Omega} \cdot \mathbf{L}_I$. Here we see that using the fast and slow fields of the staggered CP^1 representation, we obtain an expansion of the bond-fields in terms of two vector- and one scalar-field. The constraints (4.30) and (4.31) on the bond-fields are fulfilled by imposing the conditions (4.48), such that there is no condition on the scalar field φ at this stage.

Recalling that the bond-fields are related to the $\text{SO}(4)$ fields as follows:

$$\begin{aligned} \mathcal{S}_a &= s^*t_a + t_a^*s, \\ \mathcal{T}_a &= -i\varepsilon_{abc}t_b^*t_c, \end{aligned} \quad (4.52)$$

we can relate the $SO(4)$ vector-fields with the fields entering (4.51), arriving at

$$\begin{aligned}\mathcal{S} &= \mathcal{Q} - 2a^2[L_R^2 \mathcal{Q} + \varphi(\mathcal{Q} \times L_R)], \\ \mathcal{T} &= -2aL_R.\end{aligned}\quad (4.53)$$

One can easily see that the fields above fulfill the constraints obeyed by the fields $\mathcal{S}$ and $\mathcal{T}$ up to $\mathcal{O}(a^2)$.

4.2.3. Constraints and measure

The expansion (4.51) of the bond-fields in fast and slow components involves only seven components instead of eight, as originally introduced. Taking into account the first two constraints in (4.48), we are left with five fields instead of the four required to describe the degrees of freedom on a dimer formed by two $S = 1/2$ spins. Therefore, before passing to a path integral in φ , $\mathcal{Q}$, and L_R , a gauge fixing condition is still necessary. Here we choose the gauge fixing $t_3^* + t_3 = 0$. Once we proposed an expansion of the bond-fields in terms of fast and slow variables, we consider first the constraints on those variables together with the change of measure due to the transformation to these new variables.

The measure and constraints corresponding to the general gauge-fixing were obtained in Section 3.2 (Eq. (3.21)). For the particular gauge $\varphi_4 = t_3^* + t_3$ the measure can be written as follows:

$$\begin{aligned}\mathcal{DM} &= \mathcal{D}s^* \mathcal{D}s \mathcal{D}t_a^* \mathcal{D}t_a (t_3^* - t_3) \delta(t_3^* + t_3) \\ &\quad \times \delta(s^* s + t_a^* t_a - 1) \delta(s^* s^* - t_a^* t_a^*) \delta(ss - t_a t_a).\end{aligned}\quad (4.54)$$

Since we have in total seven variables given by φ , $\mathcal{Q}$, and L_R , we can eliminate one of the variables by integrating over t_3^* and imposing the constraint due to gauge fixing. Then, we have

$$\begin{aligned}\mathcal{DM} &\rightarrow \mathcal{D}s \mathcal{D}t_a^* \mathcal{D}t_a t_3 \delta(s^* s + t_1^* t_1 + t_2^* t_2 - t_3^2 - 1) \\ &\quad \times \delta(s^* s^* - t_1^* t_1 - t_2^* t_2 - t_3^2) \delta(ss - t_a t_a).\end{aligned}\quad (4.55)$$

The arguments of the δ -functions with the new variables look as follows

$$\begin{aligned}\delta(s^* s + t_1^* t_1 + t_2^* t_2 - t_3^2 - 1) &= \delta \left\{ \frac{\mathcal{Q}^2 - 1}{2} - 2ia\mathcal{Q}_3 [\varphi \mathcal{Q}_3 - (\mathcal{Q}_1 L_{R2} - \mathcal{Q}_2 L_{R1})] \right. \\ &\quad \left. - 2a^2 [(\mathcal{Q} \cdot L_R)^2 + L_R^2 (1 - \mathcal{Q}^2)] \right. \\ &\quad \left. + 2[\varphi \mathcal{Q}_3 - (\mathcal{Q}_1 L_{R2} - \mathcal{Q}_2 L_{R1})]^2 \right\}, \\ \delta(s^* s^* - t_1^* t_1 - t_2^* t_2 - t_3^2) &= \delta \left\{ \frac{\mathcal{Q}^2 - 1}{2} - 2ia \{ (1 - \mathcal{Q}^2) \varphi \right. \\ &\quad \left. + 2\mathcal{Q}_3 [\varphi \mathcal{Q}_3 - (\mathcal{Q}_1 L_{R2} - \mathcal{Q}_2 L_{R1})] \right\} \\ &\quad \left. + 2a^2 [(\mathcal{Q} \cdot L_R)^2 - (\mathcal{Q}^2 - 1)(L_R^2 + 2\varphi)] \right\}, \\ \delta(ss - t_a t_a) &= \delta \left\{ \frac{\mathcal{Q}^2 - 1}{2} - 2ia\varphi(\mathcal{Q}^2 - 1) \right. \\ &\quad \left. + 2a^2 [(\mathcal{Q} \cdot L_R)^2 - (L_R^2 + 2\varphi^2)(\mathcal{Q}^2 - 1)] \right\}.\end{aligned}\quad (4.56)$$

We can transform these constraints onto constraints on the new fields:

$$\begin{aligned} & \delta(s^*s + t_1^*t_1 + t_2^*t_2 - t_3^2 - 1)\delta(s^*s^* - t_1^*t_1 - t_2^*t_2 - t_3^2)\delta(ss - t_a t_a) \\ &= \frac{1}{J_\delta} \delta(\boldsymbol{\Omega}^2 - 1) \delta[\varphi \Omega_3 - (\Omega_1 L_{R2} - \Omega_2 L_{R1})] \delta[(\boldsymbol{\Omega} \cdot \mathbf{L}_R)^2], \end{aligned} \quad (4.57)$$

where the inverse of the Jacobian for the transformation is up to $\mathcal{O}(a^2)$

$$J_\delta^{-1} = \frac{1}{8\Omega_3} + ia \frac{\varphi}{2\Omega_3} - a^2 \frac{\varphi(2\varphi\Omega_3 + \Omega_1 L_{R2} - \Omega_2 L_{R1})}{2\Omega_3^2}. \quad (4.58)$$

On the other hand, the Jacobian for the transformation to the new fields is up to $\mathcal{O}(a^2)$

$$\begin{aligned} J &= 16\sqrt{2}(\boldsymbol{\Omega} \cdot \mathbf{L}_R) \{ \Omega_3 - 2ia[\varphi\Omega_3 + (\Omega_1 L_{R2} - \Omega_2 L_{R1})] \\ &\quad - 2a^2\varphi[\varphi\Omega_3 + (\Omega_1 L_{R2} - \Omega_2 L_{R1})] \}. \end{aligned} \quad (4.59)$$

The first factor is cancelled in going from $\delta[(\boldsymbol{\Omega} \cdot \mathbf{L}_R)^2]$ to $\delta(\boldsymbol{\Omega} \cdot \mathbf{L}_R)$. Finally, the measure in (4.55) is now

$$\mathcal{D}\mathcal{M} \propto \mathcal{D}\varphi \mathcal{D}\boldsymbol{\Omega} \mathcal{D}\mathbf{L}_R \delta(\boldsymbol{\Omega}^2 - 1) \delta\left[\varphi - \frac{(\Omega_1 L_{R2} - \Omega_2 L_{R1})}{\Omega_3}\right] \delta(\boldsymbol{\Omega} \cdot \mathbf{L}_R). \quad (4.60)$$

4.2.4. Field-theory for the spin-Peierls model

Changing notation $\mathbf{L}_R \rightarrow \mathbf{L}$, for brevity, we just express the $\text{SO}(4)$ -fields in terms of φ , $\boldsymbol{\Omega}$, and $\mathbf{L}$ using (4.52), where keeping terms up to $\mathcal{O}(a^2)$ leads to (4.53). Going back to (4.3), we can express the Hamiltonian with the new fields, leaving aside constant terms,

$$H_{\text{SP}} = \int dx \frac{Ja}{4} \left[16L^2 + (1 - \Delta) \left(\frac{1}{2} \partial_x \boldsymbol{\Omega} \cdot \partial_x \boldsymbol{\Omega} - 4\partial_x \boldsymbol{\Omega} \cdot \mathbf{L} \right) \right]. \quad (4.61)$$

Next we consider the Berry-phase as given by (4.32), where we need to consider only contribution up to $\mathcal{O}(a)$, and discard total time derivatives,

$$S_B = \int d\tau \sum_i (s^* \dot{s} + t_a^* \dot{t}_a) = -2i \int d\tau dx \mathbf{L} \cdot (\boldsymbol{\Omega} \times \partial_\tau \boldsymbol{\Omega}). \quad (4.62)$$

Finally, the total action is given by

$$\begin{aligned} S &= \int d\tau dx \left\{ -2i \mathbf{L} \cdot (\boldsymbol{\Omega} \times \partial_\tau \boldsymbol{\Omega}) \right. \\ &\quad \left. + \frac{Ja}{4} \left[16L^2 + (1 - \Delta) \left(\frac{1}{2} \partial_x \boldsymbol{\Omega} \cdot \partial_x \boldsymbol{\Omega} - 4\partial_x \boldsymbol{\Omega} \cdot \mathbf{L} \right) \right] \right\}, \end{aligned} \quad (4.63)$$

with the partition function

$$Z = \int \mathcal{D}\varphi \mathcal{D}\boldsymbol{\Omega} \mathcal{D}\mathbf{L} \delta(\boldsymbol{\Omega}^2 - 1) \delta(\boldsymbol{\Omega} \cdot \mathbf{L}) \delta\left[\varphi - \frac{(\Omega_1 L_2 - \Omega_2 L_1)}{\Omega_3}\right] e^{-S}. \quad (4.64)$$

Therefore, we can trivially integrate out φ and obtain

$$Z = \int \mathcal{D}\boldsymbol{\Omega} \mathcal{D}\mathbf{L} \delta(\boldsymbol{\Omega}^2 - 1) \delta(\boldsymbol{\Omega} \cdot \mathbf{L}) e^{-S}, \quad (4.65)$$

with the action given by (4.63). As previously done, we can integrate out $\mathbf{L}$, or what is equivalent, we solve for the saddle point for $\mathbf{L}$ as done in Section 4.1, arriving at

$$L_a = \frac{(1 - \Delta)}{8} \partial_x \Omega_a - \frac{i}{4J_1 a} \varepsilon^{abc} \Omega_b \partial_\tau \Omega_c, \quad (4.66)$$

leading to the effective action

$$\begin{aligned} \tilde{S} = \int d\tau dx \left[\frac{1}{4Ja} (\partial_\tau \boldsymbol{\Omega})^2 + \frac{Ja}{16} (1 - \Delta^2) (\partial_x \boldsymbol{\Omega})^2 \right] \\ + \frac{i}{4} (1 - \Delta) \int d\tau dx \boldsymbol{\Omega} \cdot (\partial_\tau \boldsymbol{\Omega} \times \partial_x \boldsymbol{\Omega}), \end{aligned} \quad (4.67)$$

that, as expected, coincides with the action (4.24).

5. Summary

We have presented path integral formulations for dimerized quantum antiferromagnets both for the SO(4)-algebra obeyed by the operators on a bond, as well as for bond-operators [23]. We used the formalism introduced by Faddeev and Jackiw for the quantization of constrained systems [29,30,40,43], where the presence of constraints is revealed by singular modes of the symplectic matrix resulting from the canonical form in the Lagrangian. As opposed to the Dirac treatment of constrained systems [31], no distinction among primary and secondary, first class or second class constraints is needed, but an iterative incorporation of constraints determined by the singular modes, into the canonical form. For the SO(4)-formulation, the FJ-formalism ensures that the basic brackets of the fields corresponds to those of the generators of the algebra. On the other hand, bond-operators possess a gauge degree of freedom, such that depending on the form of the gauge-fixing, different forms for the basic brackets may result, a fact that is also known from the quantization of slave-particle formulations of the t - J model [51]. As an application for both formulations, we considered the spin-Peierls model in one dimension, where we obtained the corresponding field-theories. This model, albeit simple and well known, was chosen since the gapless phase is realized due to the presence of a topological term. The present treatment shows how, by taking into account properly fluctuations in a gradient expansion, this non-trivial information is encoded in the fields appropriate for dimerized states. Since the path integral formulation presented here is not restricted by dimensionality, we expect this treatment to be useful in dealing with dimerized quantum antiferromagnets in higher dimension, as those mentioned in the Introduction.

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Appendix A. Mapping between the path integral formulations for SO(4) and bond fields

In the present appendix, we obtain the path integral representation for the SO(4) generators (Eqs. (2.36) and (2.37)) from the path integral representation for the bond fields. The starting point is Eq. (3.21)

$$\mathcal{Z} = \int \mathcal{D}s^* \mathcal{D}s \mathcal{D}t_a^* \mathcal{D}t_a (\det[M_{AB}])^{1/2} \delta[\varphi_4] \delta[\varphi_1] \delta[\varphi_2] \delta[\varphi_3] e^{-S}, \quad (A.1)$$

where the action is given by Eq. (3.22), with the constraints (3.5), (3.9), and the gauge fixing condition $\varphi_4 = t_3^* + t_3$, as in Section 4.2.3. Then, from Eq. (3.18) we have

$$(\det[M_{AB}])^{1/2} = 4(t_3 - t_3^*). \quad (\text{A.2})$$

Next, we introduced in (A.1) the SO(4) fields given by (4.52) through the identity

$$\mathbf{1} = \int \mathcal{D}\mathcal{S}_1 \mathcal{D}\mathcal{S}_2 \mathcal{D}\mathcal{S}_3 \mathcal{D}\mathcal{T}_1 \mathcal{D}\mathcal{T}_2 \mathcal{D}\mathcal{T}_3 \mathcal{P}[\mathcal{T}_3 + i(t_1^* t_2 - t_2^* t_1)], \quad (\text{A.3})$$

where $\mathcal{P}$ is a product of the remaining δ -functions that relate the SO(4) with bond-fields:

$$\begin{aligned} \mathcal{P} = & \delta[\mathcal{S}_1 - (s^* t_1 + t_1^* s)] \delta[\mathcal{S}_2 - (s^* t_2 + t_2^* s)] \delta[\mathcal{S}_3 - (s^* t_3 + t_3^* s)] \\ & \times \delta[\mathcal{T}_1 + i(t_2^* t_3 - t_3^* t_2)] \delta[\mathcal{T}_2 + i(t_3^* t_1 - t_1^* t_3)]. \end{aligned} \quad (\text{A.4})$$

It is possible to show that

$$\begin{aligned} & \mathcal{P} \delta[ss - t_\alpha t_\alpha] \delta[s^* s^* - t_\alpha^* t_\alpha^*] \\ &= \frac{1}{J} \delta\left[s^* - \left(\frac{\mathcal{S}_3}{2t_3} + it_3 \frac{\mathcal{T}_2 \mathcal{S}_1 - \mathcal{T}_1 \mathcal{S}_2}{\mathcal{S}_3^2 + \mathcal{T}_2^2 + \mathcal{T}_1^2}\right)\right] \delta\left[s + \left(\frac{\mathcal{S}_3}{2t_3} - it_3 \frac{\mathcal{T}_2 \mathcal{S}_1 - \mathcal{T}_1 \mathcal{S}_2}{\mathcal{S}_3^2 + \mathcal{T}_2^2 + \mathcal{T}_1^2}\right)\right] \\ & \times \delta\left[t_1^* + \left(\frac{t_3 \mathcal{S}_1 - is^* \mathcal{T}_2}{\mathcal{S}_3}\right)\right] \delta\left[t_1 - \left(\frac{t_3 \mathcal{S}_1 - is \mathcal{T}_2}{\mathcal{S}_3}\right)\right] \delta\left[t_2^* + \left(\frac{t_3 \mathcal{S}_2 - is^* \mathcal{T}_1}{\mathcal{S}_3}\right)\right] \\ & \times \delta\left[t_2 - \left(\frac{t_3 \mathcal{S}_2 - is \mathcal{T}_1}{\mathcal{S}_3}\right)\right] \delta\left[t_3 - i \sqrt{\frac{\mathcal{S}_3(\mathcal{S}_3^2 + \mathcal{T}_2^2 + \mathcal{T}_1^2)}{\sqrt{(\mathcal{S}_1 \mathcal{T}_1 + \mathcal{S}_2 \mathcal{T}_2)^2 + \mathcal{S}_3^2(\mathcal{S}^2 + \mathcal{T}_1^2 + \mathcal{T}_2^2)}}}\right], \end{aligned} \quad (\text{A.5})$$

where $J = -4\mathcal{S}_3(t_3 - t_3^*)$ is the Jacobian of the change of variables. Using (A.5), and after integrating over the bond-fields, we arrive at

$$\mathcal{Z} = \int \mathcal{D}\mathcal{T} \mathcal{D}\mathcal{S} \delta(\mathcal{T} \cdot \mathcal{S}) \delta(\mathcal{T}^2 + \mathcal{S}^2 - 1) e^{-\mathcal{S}}, \quad (\text{A.6})$$

where the Berry phase is given by

$$(s^* \dot{s} + t_a^* \dot{t}_a) \rightarrow \left[-\frac{\mathcal{S}_1}{\mathcal{S}_3} \dot{\mathcal{T}}_2 + \frac{\mathcal{S}_2}{\mathcal{S}_3} \dot{\mathcal{T}}_1 + \frac{1}{2} \frac{(\mathcal{T}_2 \mathcal{S}_1 - \mathcal{T}_1 \mathcal{S}_2)}{\mathcal{S}_3(\mathcal{S}_3^2 + \mathcal{T}_2^2 + \mathcal{T}_1^2)} \frac{d}{d\tau} (\mathcal{S}_3^2 + \mathcal{T}_2^2 + \mathcal{T}_1^2) \right], \quad (\text{A.7})$$

resulting in the following contributions after simplifying the expressions using the constraints of the SO(4) fields,

$$\begin{aligned} \mathcal{A}_1^{\mathcal{T}} &= \frac{\mathcal{S}_2 \mathcal{S}_3 - \mathcal{T}_2 \mathcal{T}_3}{(\mathcal{S}_3^2 + \mathcal{T}_2^2 + \mathcal{T}_1^2)}, \\ \mathcal{A}_2^{\mathcal{T}} &= \frac{-\mathcal{S}_1 \mathcal{S}_3 + \mathcal{T}_1 \mathcal{T}_3}{(\mathcal{S}_3^2 + \mathcal{T}_2^2 + \mathcal{T}_1^2)}, \\ \mathcal{A}_3^{\mathcal{T}} &= \mathcal{A}_1^{\mathcal{S}} = \mathcal{A}_2^{\mathcal{S}} = 0, \\ \mathcal{A}_3^{\mathcal{S}} &= \frac{(\mathcal{T}_2 \mathcal{S}_1 - \mathcal{T}_1 \mathcal{S}_2)}{(\mathcal{S}_3^2 + \mathcal{T}_2^2 + \mathcal{T}_1^2)}, \end{aligned} \quad (\text{A.8})$$

where the curl of the fields above only partially fulfill Eqs. (2.33) and (2.34). However, they comply with Eqs. (2.32). Using the expressions (A.8), and the expansions of the fields $\mathcal{S}$ and $\mathcal{T}$ from Eq. (4.10), we arrive at the following expression for the Berry phase:

$$\mathcal{A}^{\mathcal{T}} \cdot \partial_{\tau} \mathcal{T} + \mathcal{A}^{\mathcal{S}} \cdot \partial_{\tau} \mathcal{S} = -i \frac{1}{n_3} (\ell_1 \partial_{\tau} n_2 + \ell_1 \partial_{\tau} n_2) + \mathcal{O}(a^3). \quad (\text{A.9})$$

It is straightforward to show using the fact that $\mathbf{n}^2 = 1$ and $\mathbf{n} \cdot \boldsymbol{\ell} = 0$, that the expression above is equal to the integrand in Eq. (4.21).

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