Non linear sigma models and quantum spin systems

Antonio S. Gliozzi\textsuperscript{1,2} and Alberto Parola\textsuperscript{1,3}

\textsuperscript{1} Istituto Nazionale per la Fisica della Materia, Como
\textsuperscript{2} Dipartimento di Fisica, Universit\'a di Milano, Via Celoria 16, Milano, Italy
\textsuperscript{3} Dipartimento di Scienze Fisiche, Universit\'a dell’Insubria, Via Valleggio 11 Como, Italy

Microscopic models of quantum antiferromagnets are investigated on the basis of a mapping onto effective low energy hamiltonians. Lattice effects are carefully taken into account and their role is discussed. We show that the presence of an external staggered magnetic field modifies in a non trivial way the usual mapping onto the non linear sigma model, leading to the appearance of new terms, neglected in previous works. Our analysis is compared with Lanczos diagonalizations of $S = 1$ Heisenberg chains in a staggered field, confirming the validity of the single mode approximation for the evaluation of the dynamical structure factor. The results are relevant for the interpretation of experiments in quasi-one dimensional compounds. Microscopic realizations of SU(4) spin chains are also discussed in the framework of spin-orbital lattice systems. The low energy physics is shown to be described by sigma models with topological angle $\theta$ in one dimension. This mapping strongly suggests that the one dimensional CP\textsuperscript{3} model (with $\theta = \pi$) undergoes a second order phase transition as a function of the coupling.

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I. INTRODUCTION

Quantum spin models in low dimensionality are currently used to describe the magnetic properties of several materials including rare earths, organic compounds, transition metals and copper oxides. Available experimental data in these systems, especially magnetic resonance and neutron scattering, allow to establish the local structure as well as the most relevant features of the long range correlations. These studies generally show that magnetic materials can be accurately described by short range spin hamiltonians, at least in temperature regimes where the effects of disorder, the presence of spatial anisotropies or of dipolar interactions are negligible. The possibility to use simple spin hamiltonians to understand the physics of real systems has always been the drawing force for the development of more and more accurate methods to study the phase diagram of these models. Purely analytical techniques, like spin-waves expansions or mean field theories, have shown to be quite accurate when magnetic ordering is present. Numerical methods, based on series expansions, \textsuperscript{9} Quantum Monte Carlo simulations, \textsuperscript{10,11} or Density Matrix Renormalization Group (DMRG)\textsuperscript{12} have been successfully applied also to finite temperatures, to frustrated models and to quasi one dimensional systems, where fluctuations play a key role in determining the physics of the model. A complementary class of theoretical methods, which has been developed for investigating the effects of quantum and thermal fluctuations in many body systems, is known as the semiclassical approach and includes different techniques which have been used to provide a physical interpretation to experimental and simulation data.\textsuperscript{13}

Semiclassical theories have been widely used in framework of quantum statistical mechanics since a long time. The mapping of quantum models, in particular spin systems, onto classical effective statistical models has been extremely useful in understanding many relevant features of phase diagrams and the possible occurrence of quantum critical points. For instance, the one dimensional Ising model in a transverse magnetic field maps to the (anisotropic) two dimensional Ising model: its exact solution therefore provides a simple way to investigate the critical properties of the Ising universality class. The quantum to classical mapping can be usually justified on microscopic grounds only in the low energy and long wavelength limit, where the short range features of the original quantum model become irrelevant. Therefore, strictly speaking, the use of semiclassical methods in quantum statistical mechanics is restricted to regions characterized by a diverging correlation length and gapless low energy excitations. However, the microscopic quantum hamiltonian is often assumed to be faithfully represented by its classical counterpart in a large portion of the phase diagram provided the coupling constants present in the classical lagrangian are suitably renormalized due to quantum (short range) fluctuations.\textsuperscript{14} This expectation has been beautifully confirmed by the study of Heisenberg models in low dimensionality. In particular, exact solutions and numerical analysis of one dimensional antiferromagnets found exponentially decaying correlations and gapped excitation spectrum in integer spin chains. Conversely, semi-integer spin chains turned out to be gapless with power-law correlations. This picture fully agrees with the conjecture by Haldane, based on the presence of a topological term in the semiclassical action of one dimensional spin chains.\textsuperscript{15} Moreover, quantitative analysis of the three dimensional Non Linear Sigma Model (NL\textsuperscript{3}M) found a phase diagram which compares favorably with experiments on two dimensional antiferromagnets,\textsuperscript{16} suggesting that semiclassical approaches can be directly used for the interpretation of experimental data.

The semiclassical mapping for Heisenberg antiferro-
magnets has been also employed to study the effects of an external magnetic field on the model. Of particular physical relevance is the role of a staggered field, which directly couples to the order parameter: Such a staggered field can be realized in certain quasi-one dimensional spin one compounds where, by lowering the temperature, rare earths magnetic ions undergo a Néel transition to a three dimensional antiferromagnet which generates an alternating magnetic field acting on the Ni$^{2+}$ chains. A similar mechanism has been also invoked for the interpretation of quasi one dimensional spin one-half chains. However, the effective classical action used in the literature has not been explicitly derived from the quantum hamiltonian and we believe it should be reconsidered. In order to extract quantitative information from this NLσM a “Single Mode Approximation” (SMA) is usually adopted, but a detailed numerical study of its accuracy in this case is still missing, even if analytical studies suggest that it may be justified only for the transverse channel. In this paper, we present a microscopic derivation of the semiclassical action. We obtain an effective low energy theory different from the one commonly adopted in the literature. This theory is then analyzed in the weak and strong field limit and the results are compared to Lanczos diagonalizations.

Other magnetic materials where the use of semiclassical methods may be suggestive are spin-orbital systems, like C$\text{Fe}$ compounds or transitional metal oxides, in which orbital degeneracy is present. The special points which orbital degeneracy is present. The special points where the model has an enlarged SU(4) symmetry are particularly important in order to understand the phase diagram of the model and deserve a detailed analysis. We therefore apply the semiclassical mapping to the two microscopic models presenting this symmetry. We show that in one case the model maps straightforwardly to the CP$^3$ NLσM (with topological term in the one dimensional limit) while in the other case, we have been able to carry out the mapping only in the special case of one dimension, where again we find the same semiclassical action at a different effective coupling. Interestingly, both lattice hamiltonians have been exactly solved in D=1 with very different results: the first model has broken symmetry and gapped excitations, while in the second case it is gapless and critical. We believe that this mapping provides an important clue to the understanding of the phase diagram of CP$^n$ models, which are shown to undergo a phase transition as a function of the coupling constant.

II. SEMICLASSICAL APPROACH

In this Section we briefly review and generalize a method, proposed few years ago, for the derivation of low energy effective actions in bipartite spin systems. The main advantage of this technique, with respect to the original procedure developed by Haldane, is the possibility to keep track of lattice effects and to make direct contact with other useful microscopic approaches, like spin wave theory. The method will be later applied to Heisenberg models in an external field and to spin-orbital systems.

Be $H$ the hamiltonian of a spin model on a bipartite lattice. For instance, the celebrated Heisenberg antiferromagnet is described by

$$\mathcal{H} = \sum_{R \in B} \sum_{\delta} \mathbf{S}_R \cdot \mathbf{S}_{R+\delta}$$

where $\mathbf{S}$ are spin operators, the site index $R$ runs over the sublattice labeled by $B$ and $\delta$ is a primitive vector on the lattice connecting nearest neighbor sites. In order to evaluate the partition function $Z = Tr \exp(-\beta \mathcal{H})$ we adopt the usual coherent states formalism: we first split the interval $(0, \beta)$ in a large number $N$ of Trotter (time) slices, then insert at each imaginary time $t$ a resolution of unity based on coherent states defined at each lattice site $R$. Here we follow the standard notation $|\Omega(R,t)\rangle$: In spin $S$ models the coherent states are labeled by the unit vector $\Omega(R,t)$ and are characterized by the requirement that $\Omega \cdot S \cdot \Omega = S \Omega$. These states may be explicitly obtained by a suitable rotation in spin space of the highest eigenvector of the $S_z$ operator. The partition function can be therefore written as:

$$Z = \int \mathcal{D}\Omega(R,t) e^{-S_{eff}}$$

$$S_{eff} = \int_0^\beta dt \left[ S^2 \sum_{R \in B} \sum_{\delta} \Omega(R,t) \cdot \Omega(R+\delta,t) - \sum_R \langle \Omega(R,t) | \dot{\Omega}(R,t) \rangle \right]$$

(2)

Up to this point, the underlying lattice structure is fully present in the functional form (3) and no approximation has been introduced. However, the imaginary Wess-Zumino term

$$\langle \Omega | \dot{\Omega} \rangle = i S \frac{(\Omega \times \dot{\Omega})_z}{1 + \Omega_z}$$

(3)

prevents a simple classical interpretation of the effective action. In order to obtain a mapping onto a physically transparent classical statistical model, it is convenient to exploit the bipartite nature of the lattice by explicitly tracing out the degrees of freedom defined on sublattice $B$. This procedure can be performed analytically because the variables we are integrating out are coupled only to the classical external fields $\Omega(R,t)$ defined on the other sublattice (sublattice $A$). Therefore this step just requires the solution of the single site time dependent problem:

$$e^{-F[B(R,t)]} = Tr U_t$$

$$\frac{dU_t}{dt} = -K(R,t) U_t$$
\[ K(R, t) = S \cdot B(R, t) \]
\[ B(R, t) = S \sum_{\delta} \Omega(R + \delta, t) \]

In terms of the local free energy functional \( F[B(R, t)] \), the effective action becomes:
\[ S_{eff} = \sum_{R \in B} F[B(R, t)] - \int_0^\beta dt \sum_{R \in A} < \Omega(R, t) | \Omega(R, t) > \]

Notice that now the effective action just depends on the field \( \Omega(R, t) \) on sublattice \( A \). The solution of the problem defined in Eq. (4) can be obtained within perturbation theory for slowly varying field configurations. This requirement is satisfied in the (semiclassical) large \( S \) limit and represents the only, low energy approximation we need to introduce in the evaluation of the effective action. We notice that the lattice structure is not involved in this semiclassical analysis and the long wavelength approximation is actually unnecessary within our method. Explicitly, we obtain the following free energy functional:
\[ F[B(t)] = \int_0^\beta dt \left\{ \epsilon_0(t) + \Gamma_00(t) - \int_0^t dt' \Gamma_{01}(t) \Gamma_{10}(t') \right\} \]
\[ \Gamma_{ij}(t) = < u_i(t) | u_j(t) > \exp \left\{ \int_0^t dt' [\epsilon_i(t') - \epsilon_j(t')] \right\} \]

where \( \epsilon_i(t) \) is the \( i \)th instantaneous eigenvalue of \( K(R, t) \) and \( |u_i(t) > \) is the corresponding eigenstate. In order to obtain this expression we have assumed that the ground state of \( K(R, t) |u_0(t) > \) is non degenerate at every time \( t \). The terms shown in Eq. (4) are correct up to second order in time derivatives, as usual in semiclassical approximation. The long wavelength limit of the Berry phase term \( \Gamma_00 \) in \( F[B(t)] \) has been shown in Ref. 3 to exactly compensate the Wess-Zumino contribution in the effective action \( F[B(t)] \). As a result, the low energy and long wavelength effective action, becomes a non-linear sigma model with, possibly, a topological \( \theta \) term coming from the residual space dependence of the Berry phase \( \Gamma_00 \).

Now we are in the position to apply this method to specific lattice hamiltonians: The procedure we have just outlined requires the explicit solution of the instantaneous eigenvalue problem defined by the on site hamiltonian \( K(R, t) \) (3), the evaluation of the terms \( \Gamma_{ij}(t) \) in Eq. (4) and finally the substitution of the results into the form of the action (3).

**III. HEISENBERG MODEL IN AN EXTERNAL FIELD**

It is now established that the ground state properties and the low lying excitation spectrum of antiferromagnetic Heisenberg chains strongly depend on the value of the on site magnetic moment. Semi-integer spin chains have power law correlations and gapless spectrum while, for integer spin, correlations decay exponentially and a gap to all excitations is present \( (\Delta = 0.41048 \text{ for } S = \frac{1}{2}) \). This different behavior was first found by Haldane via a semi-classical mapping onto the O(3) non-linear \( \sigma \)-model. This conjecture was later confirmed by numerical studies based on Lanczos diagonalizations and DMRG and MC simulations.

Remarkably, these idealized models have also an experimental counterpart: neutron scattering experiment on quasi-one dimensional materials such as Ni(C2H5N)2NO2(ClO4) (NENP), confirmed that the essential physics of these systems is well described by a simple \( S = 1 \) Heisenberg hamiltonian that couples neighboring spins antiferromagnetically and takes account of the single-ion anisotropy by including an on site term \( D (S^z)^2 \). The predicted Haldane gap has been measured with great accuracy in these experiments showing good agreement with theoretical and numerical predictions.

The effects of a magnetic external perturbation on an antiferromagnetic chain, frequently gives rise to unexpected interesting phenomena. This is the case of Cu benzoate, a quasi one dimensional \( S = 1/2 \) antiferromagnet displaying a gapped excitation spectrum in an applied uniform field. Oshikawa and Affleck interpreted the experimental findings on the basis of an Heisenberg hamiltonian where spins are coupled to a weak effective staggered field. This microscopic model gives a field dependence for the gap which agrees with experimental data.

More recently, interest has been focussed on the study of the effects of external fields on \( S = 1 \) systems. In the case of a uniform magnetic field, the lowest triplet excitation states are split into a transverse and a longitudinal mode and the gap closes at a critical field \( H_c \), where Bose condensation of magnons takes place. The synthesis of compounds of the form \( R_xBaNiO_2 \) (where \( R \) stands for a magnetic rare earth) allowed to study the effects of a staggered magnetic field on the quasi-one dimensional chain of spin one Ni\(^{2+}\) ions. The magnetic moment of the Ni\(^{2+}\) couples with the R\(^{3+}\) ions that are ordered antiferromagnetically below a Néel temperature \( T_N \) (typically 16K < \( T_N < \) 80K). This three dimensional antiferromagnetic matrix generates an effective staggered magnetic field on the Ni\(^{2+}\) chains whose intensity can be tuned by varying the temperature below \( T_N \). In this way, experiments have been able to investigate the effects of a staggered field on the Haldane gap, the staggered magnetization and the susceptibility.

Stimulated by these experiments, few analytical and numerical studies attempted a theoretical analysis of spin chains in staggered fields by use of semiclassical mappings and DMRG. While qualitative agreement can be easily attained, some discrepancy still remains between the NL\( \sigma \)M approach and DMRG findings, noticeably on the form of correlation functions. This circumstance is rather surprising in light of the very nice agreement between the NL\( \sigma \)M predictions and numeri-
The strong field limit is particularly simple because, for every $S$, the ground state can be accurately described by a Néel state with gaussian transverse fluctuations. For such a problem, spin wave theory (SWT) can be applied also in one dimension giving a transverse spectrum of the form:

$$\epsilon_k = S \sqrt{\langle |\mathbf{H}| / S + 2D \rangle^2 - 4\gamma_k^2}$$

where $\mathbf{H}$ is the staggered field, $D$ is the space dimensionality and $\gamma_k = \sum_{i=1}^D \cos k_i$. To leading order, the transverse dynamical correlations in imaginary time predicted by SWT have single mode character:

$$S_{\perp}(k, \omega) = S^2 \frac{|\mathbf{H}| / S + 2(D - \gamma_k)}{\omega^2 + \epsilon_k^2}$$

The longitudinal correlations may be expressed as convolutions of the transverse ones, implying that no longitudinal branch of elementary excitations is present. According to the SWT approach, in the strong field limit, the longitudinal gap saturates at twice the transverse one.

Much more subtle is the weak field case, where quantum fluctuations strongly contrast the onset of a magnetically ordered state. In order to understand this limit, we re-examine the derivation of the NFLoM for a spin $S$ chain in an external staggered field on the basis of the method sketched in Section II.

The microscopic Hamiltonian we consider here is just the antiferromagnetic Heisenberg model in an external field $\mathbf{H}$ that can be taken either uniform or staggered:

$$\mathcal{H} = \sum_{R \in B} S_R \cdot \left[ \sum_{\delta} S_{R+\delta} + \mathbf{H} \right] \pm \mathbf{H} \cdot \sum_{R \in A} S_R$$

where the conventions are the same as in [1], and upper (lower) sign refers to uniform (staggered) applied field. Following the derivation of the previous Section, we factorize the problem in the two sublattices ($A$ and $B$) and write the effective action as:

$$S_{\text{eff}} = -\int_0^\beta dt \sum_{R \in A} \left\{ < \Omega(R, t) | \dot{\Omega}(R, t) > + S \mathbf{H} \cdot \Omega(R, t) \right\}$$

$$+ \sum_{R \in B} F[\mathbf{B}(R, t)]$$

where now

$$\mathbf{B}(R, t) = S \sum_{\delta} \Omega(R + \delta, t) + \mathbf{H}.$$ 

Therefore, we formally reduce to the same one-body problem as stated in Eq. (1). This can be solved perturbatively in the case of zero temperature ($\beta \to \infty$), and slowly varying effective fields $\mathbf{B}$. The resulting functional $F[\mathbf{B}]$ is then corrected up to second order in space and time derivatives. In this context we stress that this perturbative treatment is justified only in the low-energy limit which can be physically accessed in gapless systems. In one dimension such a requirement is satisfied in half-integer spin chains while, for integer spins, it holds only in the large $S$ limit. In fact, a perturbative renormalization group analysis, in zero external field, predicts the exponential dependence $\Delta \sim \exp(-\pi S)$. This shows that the existence of the gap is a purely quantum effect: it vanishes on approaching the classical limit ($S \to \infty$) where it is still justified to derive the effective action perturbatively also for integer spin systems. Interestingly, in the strong field limit, the one body problem can be again easily solved by considering small oscillations of the vector $\Omega$ about the direction of the magnetic field. The resulting effective action, to quadratic order in the amplitude of the oscillations, exactly reproduces all the lowest order results of SWT, including lattice effects.

Specializing Eq. (13) to the form of the effective field $\mathbf{B}$ we obtain

$$F[\mathbf{B}(R, t)] = \int_0^\beta dt \left\{ \frac{S}{2 |\mathbf{B}(R, t)|} < \mathbf{H}(R, t) \mathbf{B}(R, t) > - S |\mathbf{B}(R, t)| + \Gamma_{00} |\mathbf{m}| \right\}$$

where $\mathbf{m} = \frac{\mathbf{B}}{|\mathbf{B}|}$. The first term comes from the time integration of Eq. (1) and the second one is the ground state eigenvalue $\epsilon_0(t)$. Now we perform the continuum limit of the expression (12) assuming that the relevant configurations $\Omega(R, t)$ are slowly varying functions of space on the scale set by the lattice spacing $a$. To lowest order in spatial fluctuations we have $\mathbf{B}(R, t) = S q \Omega(R_0, t) + \mathbf{H}$ where $R_0 = R - \hat{x}$ is a reference site belonging to sublattice $A$ ($\hat{x}$ is the primitive vector pointing in the $x$ direction) and $q = 2D$ is the number of nearest neighbors of a hypercubic lattice in dimension $D$. In the weak field limit, we just need to keep terms up to second order in $\delta \mathbf{B}(R, t) = \mathbf{H} + S \sum_{x} \Omega(R + \delta, t) - \Omega(R_0, t)$. By expanding $\mathbf{m}(R, t)$ we obtain:

$$\delta \mathbf{m}(R, t) = \mathbf{m}(R, t) - \Omega(R_0, t)$$

$$= \frac{\delta \mathbf{B}(R, t)}{S q} \Omega(R_0, t) \cdot \frac{\delta \mathbf{B}(R, t)}{S q} + O(\delta B^2)$$

This leads to an approximation of the Berry phase that, to lowest order cancels the Wess-Zumino term in the effective action leaving a residual contribution:

$$\Gamma_{00} |\mathbf{m}| - \Gamma_{00} \Omega(R_0, t)$$

$$\simeq i S \delta \mathbf{m}(R, t) \cdot (\mathbf{m}(R, t) \times \mathbf{H}(R, t))$$

$$\simeq \frac{i}{q} S \delta \mathbf{m}(R, t) \cdot \Omega(R_0, t) \times \dot{\Omega}(R_0, t)$$

In one dimension, the usual topological term, arising from the spatial derivative of $\Omega$ present in $\delta \mathbf{B}$, also appears besides the contributions shown in Eq. (13). By taking the continuum limit, we finally get the form of an effective action in which one half of the degree of freedom have been integrated out:
\[ S_{\text{eff}} = \int dt \int \frac{dR}{2a^D} \left[ \frac{1}{2q} \left( \dot{\mathbf{\Omega}}(R,t) + i \mathbf{H} \times \mathbf{\Omega}(R,t) \right)^2 + a^2 S^2 |\nabla_R \mathbf{\Omega}|^2 - (1 \mp 1)S \mathbf{H} \cdot \mathbf{\Omega}(R,t) \right] + 2\pi i S Q \]  

The topological charge \( Q \) is non trivial only in \( D = 1 \) where:

\[ Q = \frac{1}{4\pi} \int dx dt \mathbf{\Omega} \cdot (\partial_x \mathbf{\Omega} \times \dot{\mathbf{\Omega}}) \]  

As a result, we obtain an effective NL\( \sigma \)M describing spin \( S \) chains in (weak) uniform (−) or staggered (+) field. The microscopic derivation allows to obtain explicit expressions for the bare spin wave velocity \( c = 2S\alpha \sqrt{D} \) and stiffness \( \rho_s = S^2a^2-D \) which coincide with those already known at \( \mathbf{H} = 0 \). While this derivation reproduces known results for a uniform field, it differs from the effective action usually quoted in the literature, where the external field only couples to \( \mathbf{\Omega} \) via the Zeeman term. It is instructive to give a simple interpretation to the formal result we have obtained: a staggered field \( \mathbf{H} \) can be written as the sum of a uniform field of the same strength minus a field twice as strong acting only on one sublattice (say the sublattice \( A \)). In this way, by tracing out the degrees of freedom living on sublattice \( B \) we obtain the same NL\( \sigma \)M action appropriate for a uniform field with the addition of a Zeeman term \( -2\mathbf{H} \cdot \mathbf{\Omega} \). This is exactly what we formally found in Eq. (15).

In order to investigate the low energy spectrum of the NL\( \sigma \)M previously obtained (13), we resort to a simple single mode approximation: the constraint \( \Omega^2 = 1 \) may be lifted through the introduction of a Lagrange multiplier \( \lambda(\mathbf{H}) \) and a linear shift of the field \( \mathbf{\Omega} \). In this way, the dynamical correlation functions in imaginary time acquire a Lorenzian form:

\[ \langle S^z_{k,\omega} S^z_{-k,-\omega} \rangle = \frac{c g S^2 / a}{\omega^2 + 2c g \lambda + c^2 k^2} \]  

\[ \langle S^\pm_{k,\omega} S^\mp_{-k,-\omega} \rangle = \frac{2c g S^2 / a}{(\omega^2 - \mathbf{H}^2) \mp 2i|\mathbf{H}| \omega + 2c g \lambda + c^2 k^2} \]  

where \( \lambda \) may be determined by a saddle point equation, or by fitting numerical data and \( g = c a^D \rho_s \). Here the \( z \) axis identifies the direction of the external field. The poles of the correlation functions directly give the dispersion relation of the model. Recalling that the NL\( \sigma \)M describes the spin degrees of freedom on a single sublattice, the wave vector \( k \) is defined modulo \( \pi \). From expressions (13) it is apparent that the correlation functions have single mode character with different dispersion relations in the transverse and longitudinal channel: In particular, at each \( k \) (modulo \( \pi \)) the transverse excitation splits into two different branches centered around the longitudinal dispersion:

\[ \Delta_L(k) = \sqrt{\Delta(\mathbf{H})^2 + c^2 k^2} \]  

\[ \Delta_T(k) = \Delta_L(k) \pm |\mathbf{H}| \]  

This form of the energy spectrum should apply to arbitrary spin \( S \) at low energy and weak staggered fields. It definitely differs from the predictions of the usual semiclassical treatments which lead, within the same single mode approximation, to spectra of the form \( \sqrt{\Delta(\mathbf{H})^2 + c^2 k^2} \) in both channels. Interestingly, also the exact solution of the 1D \( S = 1/2 \) XY model in a staggered field along the \( z \) axis shows \( \Delta_T = \Delta_L \propto H^{2/3} \). It would be interesting to study the splitting of the gap by including subleading terms in order to compare conformal field theory results with the NL\( \sigma \)M approach.

In order to ascertain the validity of the single mode approximation in one dimensional models, we performed Lanczos diagonalizations in \( S = 1 \) chains. In particular we calculated the excitation spectrum by selecting, for each \( k \), the excitation energy with the highest weight in the Lehmann representation of the dynamical correlation function.

![FIG. 1. Longitudinal (above) and transverse (below) spectral weights for \( H = 0.1 \) (full dots) and \( H = 0.01 \) (open dots) staggered field. Lanczos diagonalizations in a \( N=18 \) lattice chain. In both cases, SMA is valid near \( k = \pi \).](image-url)
creases very quickly when the staggered field is switched on: It is lowered by a factor 2.5 when the field reaches the value \( H = 0.05 \). This result should be compared with the modest decrease of the transverse spectral weight, which reduces just by 20% in the same range. Both findings agree with the reported behavior of neutron scattering data\(^3\).

In Fig. 2 the energy spectra are shown for different field strength. While at low \( H \) the spectrum is markedly asymmetrical around \( k = \pi/2 \), symmetry is restored at larger fields where it closely approaches the form predicted by SWT. Data comes from Lanczos diagonalizations performed on chains with 12, 14, 16 and 18 lattice sites.

A specific feature of our results is the splitting of two branches in the transverse excitation spectrum when a weak staggered field is applied (18). Fig. 3 shows Lanczos diagonalizations data on several \( S = 1 \) chains which provide a numerical confirmation of the semiclassical predictions. For every wavevector \( k \) we selected the longitudinal and the transverse excitation with the largest spectral weight \( Z \). When the continuum limit is appropriate, i.e. at sufficiently small \( k \) (modulo \( \pi \)), two distinct excitation branches clearly appear, differing by \( \pm |H| \) from the longitudinal excitation, in agreement with the \( \text{NLoM} \) analysis. The noticeable deviations around \( k = \pi/2 \) are clearly due to lattice effects which are not correctly reproduced in the continuum limit. Notice that finite size corrections do not seem to affect the overall structure of the excitation spectrum of the model.

In Ref.\(^3\) the DMRG technique has been applied to investigate the lowest excitations in the longitudinal and transverse channels at \( k = \pi \). The comparison of our results with DMRG is particularly instructive because it clearly shows the regimes where the use of the effective action approach is justified.

In fig. 4 we plot the quantity \( \gamma = (\Delta_L - \Delta_T)/H \) as a function of \( H \). The numerical results identify two different behaviors: at strong fields (\( H > 0.5 \)) \( \gamma \) saturates at \( \gamma = 2 \), in agreement with SWT, while in the low field limit (\( H < 0.1 \)) the splitting between the longitudinal and transverse gap quickly increases. In particular, the value \( \gamma = 1 \) predicted by our semiclassical approach

\[ \text{FIG. 2. Transverse energy gap for two different field values: } H = 0.01 \text{ (open dots) and } H = 1.0 \text{ (full dots). Lanczos diagonalizations in N=12,14,16,18 chains. In the high-field limit, the spectrum is well described by SWT (solid line).} \]

\[ \text{FIG. 3. Difference between the longitudinal and the transverse excitation spectrum for } H = 0.01 \text{ and several chain length (N=12,14,16,18). The dashed lines correspond to the theoretical prediction } \Delta_L - \Delta_T = \pm H. \]

\[ \text{FIG. 4. DMRG data: we plot the difference between the longitudinal gap and the lowest transverse excitation at } k = \pi. \text{ The data are compatible with our theoretical predictions in both the low and strong field limits.} \]
is compatible with the numerical data in the \( H \to 0 \) limit, although extended calculations in lower fields are required in order to validate our analysis.

**IV. SPIN-ORBITAL MODELS**

Spin orbital models have recently attracted considerable interest in the attempt to explain the unusual magnetic properties of a class of quasi one dimensional materials, which includes \( C_{60} \) compounds (e.g. TDAE-\( C_{60} \)) and few metal oxides (e.g. \( \text{Na}_2\text{Tl}_2\text{Sb}_2\text{O}_6, \text{Na}_2\text{V}_2\text{O}_5 \)). The physical properties of these Mott insulators are largely determined by the coupling between orbital and spin degrees of freedom which may be dominated either by Hund's rule or by dynamical Jahn-Teller effect. Possible realizations in higher dimensions are also found in fullerides or in LiNiO\(_3\). The low energy physics of these systems may be described by keeping only spin and orbital degrees of freedom. If the orbital degeneracy is twofold, like in the previous examples, the low energy model can be written in terms of two sets of spin-1/2 operators per lattice site representing respectively spin (S) and orbital (T) degrees of freedom. Usually, spin isotropy has been the subject of several studies, particularly in twofold, like in the previous examples, the low energy case, although extended calculations in lower fields are also found in higher dimensions. The general method developed in Section II can be straightforwardly applied also to this class of hamiltonians defined on bipartite lattice because the interaction just couples nearest neighbor sites. Let us discuss the two cases separately.

**A. Valence Bond model \((K = -4J)\)**

The model has four orthogonal states per site in the lattice, which correspond to the four possibilities \((\pm \frac{1}{2}, \pm \frac{1}{2})\) for the \( z \)-components of the spin and pseudospin variables. A set of coherent states is therefore labeled by a quartet of complex numbers at each site \( R \): \( z_\alpha(R) \) obeying the normalization conditions \( \sum_\alpha |z_\alpha(R)|^2 = 1 \). We follow the convention to indicate the amplitude of the \(| \uparrow, \uparrow \rangle \) state by \( z_1 \), of \(| \uparrow, \downarrow \rangle \) by \( z_2 \), of \(| \downarrow, \uparrow \rangle \) by \( z_3 \) and of \(| \downarrow, \downarrow \rangle \) by \( z_4 \). Using this representation, the partition function is written as

\[
S_{eff} = \int_0^\beta dt \left[ \sum_R z_\alpha^*(R,t) \dot{z}_\alpha(R,t) + < z(t)|H|z(t) > \right]
\]

in close analogy with Eq. (9). Summation over repeated labels \( \alpha \) is understood. Again, by tracing out sublattice B, we reduce to an effective action defined only on sublattice A, formally given by:

\[
S_{eff} = \int_0^\beta dt \sum_{R \in A} z_\alpha^*(R,t) \dot{z}_\alpha(R,t) + \sum_{R \in B} F(K(R,t))
\]

The functional \( F[K(R,t)] \) is defined by the single site problem in an external field:

\[
e^{-F[K(R,t)]} = \text{Tr} U_{R}^\beta \]

\[
\frac{dU_t}{dt} = -K(R,t) U_t
\]
where \( \mathbf{K}(R, t) \) is a \( 4 \times 4 \) matrix whose components \( K_{\mu\nu}(R, t) \) depend on the classical field \( z_\alpha(R, t) \) defined at nearest neighbor sites. The explicit form of the matrix \( \mathbf{K}(R, t) \) depends on the couplings of the Hamiltonian, and for the case we are examining is given by

\[
K_{\mu\nu}(R, t) = -J \sum_\alpha \zeta^*_{\mu}(R + \delta, t) \zeta_{\nu}(R + \delta, t)
\]

where, according to our conventions, the field \( \zeta_\alpha \) is simply related to the semiclassical variable \( z_\alpha \) by: \( \zeta_1 = z_1 \), \( \zeta_2 = -z_3 \), \( \zeta_3 = -z_2 \) and \( \zeta_4 = z_1 \). To lowest order in the spatial derivatives, i.e., taking \( z_\alpha(R, t) \sim z_\alpha(R + \delta, t) \), the instantaneous ground state of \( \mathbf{K}(R, t) \) is non degenerate and has components \( \zeta^*_{\mu}(R, t) \) with eigenvalue \( \epsilon_0 = -2DJ \) where \( D \) is the spatial dimension and we specialized to hypercubic lattices. The three other eigenvalues of \( \mathbf{K}(R, t) \) vanish and the corresponding eigenvectors are any three four dimensional vectors orthogonal to the ground state. Therefore the procedure outlined in Section II can be straightforwardly applied and requires the evaluation of \( \epsilon_0 \) to second order in the lattice spacing \( a \) (i.e., to second order in the spatial derivatives) which can be obtained by standard second order perturbation theory:

\[
\epsilon_0 = -2DJ + a^2 J \nabla(z^*_{\mu} z_{\mu}) \cdot \nabla(z_{\mu} z^*_{\mu})
\]

Moreover the coefficient \( \Gamma_{00} \) must be evaluated to first order in \( a \). The lowest order just cancels the Wess-Zumino term, while the contribution linear in \( a \) is non vanishing (for smooth configurations) only in \( D = 1 \), where it gives rise to a residual topological term:

\[
\Gamma_{00} = z_\alpha \dot{z}^*_\alpha + a \partial_x (z_\alpha \dot{z}^*_\alpha) + O(a^2)
\]

Finally, the terms \( \Gamma_{ij}(t) \) may be evaluated to lowest order in \( a \). For slowly varying fields \( z_\alpha(t) \), only the \( t' \sim t \) region does contribute to the integral in Eq. (2) leading to:

\[
\int_0^t dt' \sum_{j \neq 0} \Gamma_{0j}(t) \Gamma_{j0}(t') = -\frac{1}{2D} \left\{ \dot{z}^*_{\alpha} \dot{z}_{\alpha} - \dot{z}_{\mu} \dot{z}^*_{\mu} \dot{z}^*_{\nu} \right\}
\]

Combining the results (23,24,25) we obtain the required long wavelength limit of the effective semiclassical action for the Valence Bond SU(4) model:

\[
S_{eff} = \frac{1}{2g} \int dR \int dt \sum_{i=1}^D \sum_{\mu, \nu} |\partial_t z^*_{\mu} z_{\nu}|^2 + i\pi Q
\]

The label \( i \) runs over the \( D + 1 \) space-time coordinates and the continuum limit has been taken in the \( D \) spatial directions while the imaginary time variable has been suitably rescaled. The coupling constant \( g \) is explicitly given by

\[
g = a^{D-1} \sqrt{4D}
\]

and the topological charge \( Q \) is present only in \( D = 1 \) where it reads:

\[
Q = \frac{1}{2\pi i} \int dx dt \partial_x (z_\alpha \dot{z}^*_\alpha)
\]

Tracing out a sublattice is an efficient way to take into account the short range antiferromagnetic correlations present in the model leading to an effective action describing the much smoother fluctuations on a single sublattice. In order to support this interpretation of the procedure we have adopted, Fig. (5) shows the magnetic structure factor obtained by Lanczos diagonalization on a 16-site lattice: The sharp peak at wavevector \( k = \pi \) confirms that the most relevant correlations have indeed periodicity of two lattice spacing.

The formal construction of the effective action for the Valence Bond SU(4) model shows that the long wavelength and low energy physics is described by a \( D + 1 \) dimensional NL\( \sigma \)M or CP\(^3\) model (with topological angle \( \theta = \pi \) in \( D = 1 \) ). The known exact solution of the lattice model in one dimension implies that the CP\(^3\) model at \( g = 2 \) has correlations exponentially decaying in space-time. Moreover, the spin model is known to develop dimer order in the thermodynamic limit, which implies breaking of translational invariance by a lattice spacing together with breaking of parity. In going to the continuum limit, one sublattice has been traced out and then the CP\(^3\) model remains translationally invariant but parity breaking should still occur. This picture is supported by Lanczos diagonalizations of the spin model showing that the quantum numbers of the two SU(4) singlet states which collapse in the thermodynamic limit correspond to momenta \( P = 0 \) and \( P = \pi \) and opposite parity (i.e., reflections through a lattice site). Clearly, the mapping we have developed neglects cut-off effects and holds only for sufficiently smooth configurations of the classical field. Therefore, the resulting estimate of the bare coupling constant \( g = 2 \) should be taken with caution but we are confident that the qualitative behavior of the CP\(^3\) model does indeed capture the physics of this lattice spin system, analogously to the familiar SU(2) case.

The Valence Bond model we have considered belongs to the SU(n) class already studied by Affleck, Read and Sachdev by use of 1/n expansion. These analyses show that the ground state breaks parity and translational symmetry and may be described by a Valence Bond Solid (VBS) in one dimension, at least for sufficiently large \( n \). The exact solution of the Valence Bond model confirms that this picture holds down to \( n = 4 \). The two dimensional case is more difficult: in the \( n \to \infty \) limit the system has infinite degeneracy and can be represented as an arbitrary covering of the lattice by nearest neighbor valence bonds. This degeneracy is lifted at leading order in 1/n giving rise to a (plaqette) resonating valence bond solid. In fact, the model maps onto a dimer Hamiltonian which has been studied by Monte Carlo techniques. However, diagonal-
izations and Quantum Monte Carlo simulations directly performed on the hamiltonian \[ (19) \] suggest that the ground state might be a spin liquid at \( n=4 \) and therefore argue in favor of a phase transition between magnetically disordered phases as a function of \( n \).

![Graph](image)

**FIG. 5.** Magnetic structure factor for the two SU(4) models considered here. Lanczos data for a 16-site chain with periodic boundary conditions. Full dots: \( K = -4J \) model. Open dots: \( K = 4J \) model.

**B. Sutherland model \( (K = +4J) \)**

The derivation of the NLs\( \sigma \)M appropriate for the second SU(4) point of the spin hamiltonian \[ (13) \] can be carried out following the same procedure adopted before and leading to Eqs. \[ (20) \] and \[ (21) \]. However, the associated quantum mechanical problem \[ (22) \] is now defined by the slightly different 4 \( \times \) 4 matrix

\[
K_{\mu\nu}(R, t) = J \sum_\delta z_\mu(R + \delta, t) z_\nu^*(R + \delta, t)
\]

instead of Eq. \[ (20) \]. To leading order in spatial fluctuations, we can set \( z_\mu(R + \delta) \sim z_\mu(R) \). In this case, the (instantaneous) ground state of the one site problem defined by the matrix \[ (20) \] is threefold degenerate. As a result, we cannot carry out straightforwardly the trace over one sublattice, suggesting that this procedure is not able to eliminate the long range oscillations in spin correlations. In turn, this means that the continuum limit cannot be taken just by considering the spin configurations on a single sublattice, as in usual antiferromagnets and larger primitive cells must be taken into account. A confirmation of such an interpretation comes from Lanczos diagonalizations on this model: as shown in Fig. 4, in one dimension the spin correlations displays oscillations characterized by the wavevector \( k = \pi/2 \), implying a four site periodicity. This suggests a generalization of the procedure sketched in Section II: instead of tracing out one sublattice, we now keep one site every four sites of the chain. Therefore we need the solution of a three site problem, defined by the hamiltonian \[ (14) \], with “time” dependent boundary conditions defined by the classical field \( z_\alpha(R, t) \) on the two adjacent sites. Equation \[ (20) \] is basically unchanged, but now the sublattice \( A \) includes only one fourth of the sites of the chain and the free energy functional \( F \) is defined by Eq. \[ (22) \] in terms of a matrix \( K \) acting on a Hilbert space of dimension 64. To lowest order in spatial fluctuations of the classical field \( z_\alpha(R, t) \), the full spectrum of \( K \) can be explicitly obtained by solving the eigenvalue equation:

\[
J \left[ z_\mu z_\nu^* u_{\alpha,\nu,\lambda} + u_{\nu,\lambda,\alpha} + z_\lambda z_\alpha^* u_{\mu,\nu,\alpha} \right] = \epsilon u_{\mu,\nu,\lambda}
\]

In particular, the ground state wavefunction of the quantum problem is now non-degenerate and reads

\[
u_{\mu,\nu,\lambda} = \frac{1}{\sqrt{6}} z_\mu^* \epsilon_{\alpha\mu\nu}
\]

where \( \epsilon_{\alpha\mu\nu} \) is the fully antisymmetric Levi-Civita tensor. The corresponding eigenvalue is simply \( \epsilon_0 = -2J \), while the Berry phase contribution gives

\[
\Gamma_{00} = \frac{1}{6} z_\alpha \epsilon_{\alpha\mu\nu} \frac{\delta}{\delta t} \epsilon_{\beta\mu\nu} = z_\alpha \frac{\delta}{\delta t} z_\alpha^*
\]

and cancels the Wess-Zumino term in the effective action. In order to obtain a non-trivial theory we have to include long wavelength fluctuations of the classical field \( z(R, t) \). This can be done by use of perturbation theory in the associated quantum three site problem. The solution is sketched in Appendix where the required terms are explicitly evaluated. Here we just quote the final result, after having taken the continuum limit: The spin fluctuations on the sublattice are described by a NLs\( \sigma \)M which coincides with the one obtained for the Valence Bond model \[ (27) \] at a bare coupling

\[
g = \frac{6}{\sqrt{5}}
\]

larger than the estimate \( g = 2 \) obtained in one dimension for the Valence Bond model \[ (28) \]. Also for this hamiltonian the topological angle \( \theta \) is given by \( \theta = \pi \).

As previously stressed, the Sutherland model is critical in one dimension, with power law correlations characterized by oscillations of period 4\( a \) corresponding to a characteristic wavevector \( k = \pi/2 \), as also confirmed by the Lanczos diagonalization results shown in Fig. 3. If the mapping onto a CP\( ^3 \) theory (with topological angle \( \theta = \pi \)) faithfully describes the long wavelength physics of the lattice model, we conclude that the CP\( ^3 \) action in 1 + 1 dimension has correlations

\[
< z_\alpha^*(0, 0) z_\beta(0, 0) z_\beta^*(x, t) z_\alpha(x, t) > \sim (x^2 + t^2)^{-3/4}
\]
On the other hand, the exact solution of the Valence Bond hamiltonian together with the semiclassical mapping of Section IV-A implies that the CP$^3$ model has exponentially decaying correlations at $g = 2$. These two results may be reconciled if we assume that the CP$^3$ theory in $1+1$ dimension undergoes a second order phase transition as a function of the coupling $g$ and the Sutherland model describes the physics at the critical point. Another possibility would be the occurrence of a gapless phase in the model, like in the celebrated CP$^3$ case. This alternative explanation, however, conflicts with available analytical and numerical evidence pointing towards a massive regime at strong coupling. A phase transition in the CP$^3$ model cannot be related to a spontaneous breaking of the continuous SU(4) symmetry while a possibility would be the occurrence of a gapless phase in 1 + 1 dimension. Of course the estimate (34) we have obtained for the critical coupling will be renormalized by finite cut-off effects but the overall picture of the phase diagram emerging from the semiclassical analysis should be robust. This result may have implications in the framework of the strong CP problem in field theory.

V. CONCLUSIONS

In this paper we discussed some application of the semiclassical approach to spin systems in low dimensionality. This technique is known to capture the qualitative features of quantum models and to provide a useful framework for the interpretation of experimental and numerical data.

For Heisenberg chains in a staggered field we pointed out some difficulty and inconsistency of usual treatments, especially in the weak field limit, where the structure of the effective NLσM turns out to be richer than expected. The general form of the excitation spectrum predicted by semiclassical approaches has been confirmed by use of Lanczos diagonalizations in finite clusters which also provide some support to the usually adopted SMA. Our results are fully compatible with existing DMRG data and show that different physical regimes occur in the phase diagram of this model. A recent DMRG investigation of a $S = 2$ spin chain also pointed out a similar behavior.

The new NLσM we derived is expected to represent only the low field region while, for moderate/high staggered fields, simple perturbative approaches, like spin wave theory, are fully adequate to describe the excitation spectrum of the model. It seems unlikely that a single effective action in the continuum limit might be able to encompass these two very different physical behaviors.

A semiclassical analysis of spin-orbital models characterized by a SU(4) symmetry has also been performed in two different regimes. In one case we straightforwardly obtained, in the long wavelength limit, a mapping to the CP$^3$ NLσM describing the fluctuations of spin-orbital degrees of freedom on the same sublattice.

Recent numerical simulations argued in favor of a disordered ground state in such a model for $D = 2$, while in one dimension the exact solution of the lattice hamiltonian proved that spontaneous dimerization occurs. In the other SU(4) model we have examined, a smooth continuum limit requires a coarse graining over several lattice sites, suggesting that the relevant fluctuations are characterized by a wavevector $k$ different from the antiferromagnetic one. We explicitly performed the analysis only for the one dimensional model, where we again obtained the same CP$^3$ model which now describes fluctuations about $k = \pi/2$. The phase diagram of such a NLσM has been extensively studied, particularly in $1+1$ dimension, in connection to the CP problem in field theory. Several proposals have been put forward in the literature, including spontaneous parity breaking and deconfining transition. The long wavelength mapping between spin chains and two dimensional field theories may provide a clue for the final understanding of the phase diagram of the CP$^3$ model, analogously to what has been found for the Wess Zumino Witten model.

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VI. APPENDIX

In this appendix we briefly illustrate the procedure adopted for the analytical solution of the generalized three site problem

$$J \sum_{\mu,\lambda,\nu} \alpha \beta \gamma 
\left( \delta_{\mu,\nu,\lambda} u_{\alpha,\nu,\lambda} + u_{\mu,\lambda,\nu} + \right. \left. \delta_{\lambda,\mu,\nu} u_{\alpha,\nu,\lambda} \right) = \epsilon u_{\mu,\nu,\lambda}$$

(36)

up to second order in the lattice spacing $a$. Here $z_{\alpha} = z_{\alpha} + 4a \partial_{x} z_{\alpha} + 8a^{2} \partial_{x}^{2} z_{\alpha} + O(a^{3})$. We employ standard second order perturbation theory which gives

$$\Delta \epsilon = < u_{0} | \Delta K | u_{0} > + \sum_{n \neq 0} \frac{< u_{0} | \Delta K | u_{n} >^{2}}{\epsilon_{n} - \epsilon_{0}}$$

(37)

The unperturbed eigenvectors $| u_{n} >$ are the solutions of the eigenvalue equation (35) and $\epsilon_{n}$ are the corresponding eigenvalues. The ground state $| u_{0} >$ is explicitly given in Eq. (36) and $\epsilon_{0} = -2J$. Due to the manifest SU(4) invariance of the eigenvalue equation, the external field $z_{\alpha}$ may be chosen to point in the “1” direction without loss of generality: $z_{\alpha} = \delta_{\alpha,1}$. The lowest order term gives:

$$< u_{0} | \Delta K | u_{0} > = \frac{16}{3} a^{2} J \left[ (z_{1}^{*} \partial_{x} z_{1})^{2} - \partial_{x} z_{1} \partial_{x} z_{1}^{*} \right]$$

(38)

while the sum over excited states which appears at second order requires the evaluation of the matrix element

$$< u_{0} | \Delta K | u_{n} > = \frac{4aJ}{\sqrt{6}} \epsilon_{1,\alpha,\nu} u_{\mu,\nu,1} \partial_{x} z_{\alpha}$$

(39)
for a generic excited state $u_{\mu \nu 1}$. The only solutions of the unperturbed eigenvalue equation \( \{ \} \) which give a non vanishing contribution are those corresponding to the eigenvalue $\epsilon = \pm \sqrt{2} J$ and $\epsilon = 0$. The former states are given by $u_{123} = u_{231} = -u_{132} = -u_{213} = \pm u_{312}/\sqrt{2} = \mp u_{213}/\sqrt{2} = 1/\sqrt{8}$. The latter states are $u_{123} = u_{321} = -u_{132} = -u_{213} = 1/2$ Both excited states are three times degenerate: the other states being obtained by cyclic permutations of the labels (234). Inserting these results into the perturbative expansion \( \{ \} \) we get:

\[
\Delta \epsilon = -\frac{4}{3} J a^{2} \left[ \left( z_{\alpha}^{*} \partial_{z} z_{\alpha} \right)^{2} - \partial_{z} z_{\alpha} \partial_{z} z_{\alpha}^{*} \right]
\]

(40)

The last required step is the evaluation of the Berry phase term $\Gamma_{0}$ to first order in the lattice spacing. Again, by use of perturbation theory, we get

\[
\Gamma_{00} = \langle u_{0} | \hat{a}_{0} > + 2 \text{Im} \sum_{\mathbf{n} \neq 0} \frac{\langle u_{0} | \Delta K | u_{n} >}{\epsilon_{0} - \epsilon_{n}} < u_{n} | \hat{a}_{0} >
\]

(41)

The intermediate states which contribute to the sum are those corresponding to $\epsilon = \pm \sqrt{2} J$ which give:

\[
\Gamma_{00} = z_{\alpha} z_{\alpha}^{*} - 2a \partial_{z} (z_{\alpha}^{*} z_{\alpha})
\]

(42)

This, in turn, gives the well known topological term quoted in the text \( \{ \} \).

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