Semiclassical description of Heisenberg models via spin-coherent states

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Abstract. We use spin-coherent states as the basis of a time-dependent variational *ansatz* for a semiclassical description of a large family of Heisenberg models. In addition to following common approaches we also evaluate the square variance $\langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2$ of the Hamiltonian in terms of coherent states. This quantity turns out to have a natural interpretation with respect to time-dependent solutions of the equations of motion and allows an estimate of quantum fluctuations in a semiclassical regime to be made. The general results are applied to solitons, instantons and vortices in several one- and two-dimensional models.

1. Introduction

There has been a lot of work on classical spin systems in the last few decades, commonly using a continuum description; for a review, see Kosevich *et al* (1990). Some one-dimensional models have been identified as integrable and treated by means of the inverse scattering method (Takhtajan 1977, Fogedby 1980, Sklyanin 1979). A common feature of such non-linear evolution equations is the existence of localized solutions like solitary waves and, in the integrable case, mathematical solitons.

For quantum spin systems, analytical treatments appear to be restricted to one-dimensional models. For the spin-$\frac{1}{2}$ Heisenberg chain of N lattice sites, Bethe (1931) managed to reduce the problem of the diagonalization of the Hamiltonian acting on a 2^N-dimensional Hilbert space to the problem of solving N coupled non-linear algebraic equations, which are well understood in the thermodynamic limit. By means of this Bethe *ansatz* and its algebraic formulation, many properties of the model such as thermodynamic quantities could be extracted. Nevertheless, the eigenstates of the Hamiltonian themselves are obtained only rather implicitly and are naturally translationally symmetric, i.e. non-localized. Thus, a quantum analogue to a classical time-dependent soliton, which should be not an eigenstate of the energy but a superposition of such eigenstates, has not been found yet.

So it is desirable to give a description of solitons in the semiclassical regime, i.e. for large but finite values of the spin length. Considerable work in this direction has been done using different kinds of bosonization and tensor products of coherent oscillator states as a variational *ansatz*; see, e.g., de Azevedo *et al* (1982), Ferrer and Pozo (1988), Kapor *et al* (1990). The disadvantages of these methods include the difficulties in treating infinite series of non-trivial operator products and, more fundamental, the problem of mapping the finite-dimensional Hilbert space of a spin onto an infinite-dimensional bosonic space.

An alternative to such approaches is that based on spin-coherent states as introduced by Radcliffe (1971). Balakrishnan and Bishop (1985, 1989) and Balakrishnan *et al* (1990)

used these objects for treating ferromagnetic Heisenberg chains and evaluated quantum corrections to classical soliton dispersion laws. In detail, their way of proceeding has been subject to some criticism by Haldane (1986), but the general findings concerning soliton stability with respect to quantum fluctuation seem to be valid and will be confirmed in the present work. Moreover, Frahm and Holyst (1989) suggested an extension of spin-coherent states introducing a squeezing similar to that used on bosonic states. Unfortunately, this approach leads for generic models to very complicated equations of motion for the classical angular variables and the additional squeeze parameter, which cannot be solved exactly for non-trivial cases.

In this paper we follow the above authors and use (unsqueezed) spin-coherent states as a variational *ansatz* for a large family of Heisenberg models. In addition to the quantities considered in the above references, we also calculate the quantum mechanical variance of the energy. This quantity can be used as a test of the validity of the approach; on the other hand, the general expression obtained has a natural physical interpretation concerning energy fluctuations in time-dependent spin structures. Finally we apply our results to several important solitary solutions of spin models.

2. Coherent states

For the Hilbert space of a spin of length S, we define a spin-coherent state $|S; \vartheta, \varphi\rangle$ by the equation

$$s_{\vartheta,\varphi} \cdot \hat{S}|S; \vartheta, \varphi\rangle = \hbar S|S; \vartheta, \varphi\rangle \tag{1}$$

for the direction $s_{\vartheta,\varphi} = (\sin \vartheta \cos \varphi, \sin \vartheta \sin \varphi, \cos \vartheta)$. In the usual basis of eigenstates of $\hat{S}^z$ ($\hat{S}^z|m\rangle = \hbar m|m\rangle$), these states can be expressed as

$$|S; \vartheta, \varphi\rangle = U(\vartheta, \varphi)|S\rangle = \sum_{n=0}^{2S} \binom{2S}{n}^{1/2} \left(\cos\left(\frac{\vartheta}{2}\right)\right)^{2S-n} \left(\sin\left(\frac{\vartheta}{2}\right)\right)^n e^{i\varphi(n-S)}|S-n\rangle \tag{2}$$

with

$$U(\vartheta, \varphi) = \exp\left(-\frac{i}{\hbar}\varphi \hat{S}^z\right) \exp\left(-\frac{i}{\hbar}\vartheta \hat{S}^y\right). \tag{3}$$

Clearly, we have $\langle S; \vartheta, \varphi|\hat{S}|S; \vartheta, \varphi\rangle = \hbar S s_{\vartheta,\varphi}$, but, in the expectation values of higher products of spin components, contributions of different order in the spin length S arise. A list of diagonal elements useful in the following is given in appendix A, where we also demonstrate how to take the classical limit of such expressions.

The spin-coherent states have the minimum-uncertainty product

$$\Delta(e_1 \cdot \hat{S})\Delta(e_2 \cdot \hat{S}) = \frac{\hbar}{2}\Delta(e_3 \cdot \hat{S}) \tag{4}$$

with $\Delta(\hat{O})$ being the variance of an operator $\hat{O}$ and e_1, e_2, e_3 an orthonormal system. Furthermore, they fulfil the (over-) completeness relation

$$\frac{2S+1}{4\pi} \int_0^{2\pi} d\varphi \int_0^\pi d\vartheta \ \sin \vartheta |S; \vartheta, \varphi\rangle\langle S; \vartheta, \varphi| = \mathbf{1}. \tag{5}$$

Nevertheless, it should be mentioned that, for an arbitrary linear combination of coherent states, a direction $s_{\vartheta,\varphi}$ solving equation (1) cannot be found. Therefore the spin-coherent states do not form a subspace of the Hilbert space, but a submanifold diffeomorphic to the two-dimensional unit sphere. Only in the case where $S = \frac{1}{2}$ can every (normalized) state vector be identified as a coherent state.

3. The time-dependent variational method

Let us consider the following class of one-dimensional spin models:

$$\mathcal{H} = \sum_n \sum_{i=1}^{3} \left[\alpha_i \hat{S}_n^i \hat{S}_{n+1}^i + \beta_i \hat{S}_n^i \hat{S}_n^i + \gamma_i \hat{S}_n^i \right]. \tag{6}$$

The index i runs over the three spatial directions x, y, z. Each lattice site labelled by n carries a spin of uniform length S. The Hamiltonian includes an anisotropic exchange coupling between nearest neighbours, a local anisotropy and a magnetic field. The parameters α_i, β_i, γ_i may be chosen arbitrarily, in particular as regards their sign.

We now employ the direct product of coherent states

$$|\psi(t)\rangle = \bigotimes_n |S; \vartheta_n, \varphi_n\rangle \tag{7}$$

as a time-dependent variational *ansatz*, i.e. we assume the time evolution of the state $|\psi(t)\rangle$ under the above Hamiltonian to be given in terms of time-dependent functions $\vartheta_n(t)$, $\varphi_n(t)$. With $\langle\ \rangle$ denoting an expectation value within (7), $s_n = (\sin\vartheta_n\cos\varphi_n, \sin\vartheta_n\sin\varphi_n, \cos\vartheta_n)$ and cartesian directions e^i, we have for $\mathcal{H}$

$$\langle\mathcal{H}\rangle = (\hbar S)^2 \sum_n \sum_{i=1}^{3} \left[\alpha_i (s_n \cdot e^i)(s_{n+1} \cdot e^i) + \left(1 - \frac{1}{2S}\right)\beta_i (s_n \cdot e^i)^2 + \frac{\gamma_i}{\hbar S}(s_n \cdot e^i) \right] \tag{8}$$

and from the Heisenberg equations of motion

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{S}_n = -\frac{\mathrm{i}}{\hbar}[\hat{S}_n, \mathcal{H}]$$

we have

$$\frac{\mathrm{d}}{\mathrm{d}t}s_n = (\hbar S)\sum_{i=1}^{3}\left[\alpha_i(s_n \times e^i)[(s_{n-1} + s_{n+1}) \cdot e^i] + 2\left(1 - \frac{1}{2S}\right)\beta_i(s_n \times e^i)(s_n \cdot e^i) \right.$$
$$\left. + \frac{\gamma_i}{\hbar S}(s_n \times e^i) \right]. \tag{9}$$

The quantity $\hbar S$ becomes the classical spin length in the limit $S \to \infty$, $\hbar \to 0$, $\hbar S = \text{constant}$. Equations (8) and (9) are identical to the classical energy and the Landau–Lifshitz equation up to a renormalization of the local anisotropy by a factor of $1 - 1/(2S)$, reflecting the fact that this term does not contribute to the dynamics for $S = \frac{1}{2}$. Therefore the variational *ansatz* provides semiclassical corrections to the equation of motion and reproduces the correct classical limit. This property of spin-coherent states has been found by several authors previously to hold for particular spin models (see, e.g., the references given in the introduction), and is proved in appendix B to hold for an arbitrary Hamiltonian.

Next we examine the square variance of the Hamiltonian, i.e. $\langle\mathcal{H}^2\rangle - \langle\mathcal{H}\rangle^2$. This quantity is non-zero only in the quantum case and (like $\langle\mathcal{H}\rangle$) is strictly an invariant of the system, whatever the exact quantum mechanical time evolution of the state (7) is. After extensive algebra one ends up with the following expression:

$$\langle\mathcal{H}^2\rangle - \langle\mathcal{H}\rangle^2 = (\hbar S)^4 \sum_n \left[\frac{1}{2S}\left(\sum_{i=1}^{3}\left[\alpha_i(s_n \times e^i)[(s_{n-1} + s_{n+1}) \cdot e^i] \right.\right.\right.$$
$$\left.\left.\left. + 2\left(1 - \frac{1}{2S}\right)\beta_i(s_n \times e^i)(s_n \cdot e^i) + \frac{\gamma_i}{\hbar S}(s_n \times e^i) \right]\right)^2 \right.$$

$$+ \frac{1}{8S^2}\bigg(\sum_{i,j=1}^{3}[\alpha_i\alpha_j([(\boldsymbol{s}_n \times \boldsymbol{e}^i) \cdot (\boldsymbol{s}_n \times \boldsymbol{e}^j)]$$

$$\times [(\boldsymbol{s}_{n-1} \times \boldsymbol{e}^i) \cdot (\boldsymbol{s}_{n-1} \times \boldsymbol{e}^j) + (\boldsymbol{s}_{n+1} \times \boldsymbol{e}^i) \cdot (\boldsymbol{s}_{n+1} \times \boldsymbol{e}^j)]$$

$$- [\boldsymbol{s}_n \cdot (\boldsymbol{e}^i \times \boldsymbol{e}^j)][(\boldsymbol{s}_{n-1} + \boldsymbol{s}_{n+1}) \cdot (\boldsymbol{e}^i \times \boldsymbol{e}^j)])]$$

$$+ 2\sum_{i,j=1}^{3}\bigg[\bigg(1 - \frac{1}{2S}\bigg)\beta_i\beta_j((\boldsymbol{s}_n \times \boldsymbol{e}^i)^2(\boldsymbol{s}_n \times \boldsymbol{e}^j)^2 - [\boldsymbol{s}_n \cdot (\boldsymbol{e}^i \times \boldsymbol{e}^j)]^2)\bigg]\bigg)\bigg].$$

$$(10)$$

The square variance of the energy consists essentially of two contributions of order $1/S$ and $1/S^2$ respectively. In the above summation over the lattice sites the squared expression in the term of order $1/S$ can be recognized as the r.h.s. of equation (9). Thus, we have

$$\langle\mathcal{H}^2\rangle - \langle\mathcal{H}\rangle^2 = (\hbar S)^2 \sum_n \frac{1}{2S}\bigg(\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{s}_n\bigg)^2 + \mathrm{O}\bigg(\frac{1}{S^2}\bigg). \qquad (11)$$

Within our variational approach, the leading order of the quantum fluctuations of the energy is purely due to the time dependence of the state vector. On the other hand, for a quantum state which has a non-trivial time evolution and is consequently not an eigenstate of the Hamiltonian, the energy must definitely have a finite uncertainty. Following this observation, the leading term in (11) is certainly not an artifact of the *ansatz* (7), and in fact it is a physically relevant expression for the energy fluctuations in time-dependent semiclassical spin structures. So we have found good evidence that the *ansatz* based on the spin-coherent states not only reproduces the classical limit but is still meaningful for a semiclassical description. The contributions of order $1/S^2$ in (10) cannot be interpreted in a general way and should be studied in the context of particular models. We will see that these terms can often be considered as a criterion for the validity of the variational method.

For brevity we have concentrated in (6) on a one-dimensional model. For higher dimensions one simply has to infer the appropriate number of neighbours of each lattice site in the summations. The result can always be written in the form (11). Moreover, it is also straightforward to see that the result (11) is still valid in the case of exchange couplings of longer range.

Thus, our above findings apply to a large variety of (ferromagnetic or antiferromagnetic) spin models in arbitrary dimensions. This will be illustrated in the next section for several one- and two-dimensional ferromagnetic models.

4. Application to solitons, instantons and vortices

We now calculate the quantum mechanical energy uncertainty for solitary solutions within different Heisenberg models. We denote the leading order in $1/S$ by Ω_1 (cf. equation (11)) and the remaining contributions by Ω_2, i.e. $\langle\mathcal{H}^2\rangle - \langle\mathcal{H}\rangle^2 = \Omega_1 + \Omega_2$.

(i) A ferromagnetic Heisenberg chain with isotropic exchange coupling and an external field is given by

$$\mathcal{H}_1 = -J\sum_n\bigg[\hat{\boldsymbol{S}}_n \cdot \hat{\boldsymbol{S}}_{n+1} + \hat{\boldsymbol{S}}_n \cdot \boldsymbol{B}\bigg] \qquad (12)$$

with $J > 0$. Equations (8)–(10) read

$$\langle\mathcal{H}_1\rangle = -(\hbar S)^2 J\sum_n\bigg[\boldsymbol{s}_n \cdot \boldsymbol{s}_{n+1} + \boldsymbol{s}_n \cdot \frac{\boldsymbol{B}}{\hbar S}\bigg] \qquad (13)$$

$$\frac{d}{dt} s_n = (\hbar S) J \left(s_n \times (s_{n-1} + s_{n+1}) + s_n \times \frac{B}{\hbar S} \right) \tag{14}$$

$$\langle \mathcal{H}_1^2 \rangle - \langle \mathcal{H}_1 \rangle^2 = (\hbar S)^4 J^2 \sum_n \left[\frac{1}{2S} \left(s_n \times (s_{n-1} + s_{n+1}) + s_n \times \frac{B}{\hbar S} \right)^2 \right.$$
$$\left. + \frac{1}{8S^2} [(1 - s_n \cdot s_{n-1})^2 + (1 - s_n \cdot s_{n+1})^2] \right]. \tag{15}$$

We choose appropriate units with $J = 1$, $\hbar S = 1$, and the lattice spacing $a = 1$ and calculate the expectation value of (12) in the usual continuum approximation for an infinite system:

$$\langle \mathcal{H}_1 \rangle = \int d\xi \, \left(\frac{1}{2} \left(\frac{(\partial_\xi p)^2}{1 - p^2} + (1 - p^2)(\partial_\xi q)^2 \right) - Bp \right) \tag{16}$$

where we have put the magnetic field in the z-direction, subtracted the ground-state energy and introduced the canonical conjugate fields $p = \cos \vartheta$, $q = \varphi$; ξ denotes the spatial variable in the chain direction. The equations of motion (14) read in the continuum approximation

$$\partial_t q = -\frac{1}{1 - p^2} \partial_\xi^2 p - \frac{p}{(1 - p^2)^2} (\partial_\xi p)^2 - p(\partial_\xi q)^2 - B \tag{17}$$

$$\partial_t p = (1 - p^2) \partial_\xi^2 q - 2p(\partial_\xi p) \partial_\xi q. \tag{18}$$

These equations have well-known soliton solutions (Tjon and Wright 1977):

$$p(\xi, t) = 1 - \frac{2}{(B + \omega)\Gamma^2} \text{sech}^2 \left(\frac{\xi - vt - \xi_0}{\Gamma} \right) \tag{19}$$

$$q(\xi, t) = q_0 + \omega t + \frac{v}{2}(\xi - vt - \xi_0) + \tan^{-1} \left(\frac{2}{v\Gamma} \tanh \left(\frac{\xi - vt - \xi_0}{\Gamma} \right) \right) \tag{20}$$

with the soliton width

$$\Gamma = \frac{1}{\sqrt{B + \omega - v^2/4}} > 0 \tag{21}$$

and ξ_0, q_0 being constants. The above solution is a pulse soliton with velocity v and an internal frequency ω constrained by (21). Its energy is calculated from (16):

$$E = \frac{4}{\Gamma} + \frac{B}{B + \omega} \frac{4}{\Gamma}. \tag{22}$$

The square variance $\langle \mathcal{H}_1^2 \rangle - \langle \mathcal{H}_1 \rangle^2 = \Omega_1 + \Omega_2$ can be obtained from the continuum version of (15):

$$\Omega_1 = \frac{1}{S} \left(\frac{1}{\Gamma} \left(8(2B + 3\omega) + \frac{4\omega^2}{B + \omega} \right) - \frac{1}{\Gamma^3} \left(16 + \frac{8\omega^2}{3(B + \omega)^2} + \frac{8\omega}{B + \omega} \right) \right) \tag{23}$$

$$\Omega_2 = \frac{1}{S^2} \frac{4}{3\Gamma^3} \tag{24}$$

where (21) has been used. As explained in the previous section, the quantity Ω_1 can be interpreted as a natural property of a time-dependent spin state in the semiclassical regime. As a criterion for the importance of quantum effects absent from our *ansatz* (7) we compare Ω_2 with the soliton energy, i.e.

$$\frac{\sqrt{\Omega_2}}{E} = \frac{1}{S\sqrt{\Gamma}} \frac{B + \omega}{2\sqrt{3}(2B + \omega)}. \tag{25}$$

We see that higher-order quantum corrections to our variational approach are negligible for solitons with large width and consequently small energy. If this condition is not fulfilled the spin length S becomes significant, in agreement with the work of Balakrishnan and Bishop mentioned in the introduction.

The continuum approximation is a good description of the system if the classical fields p, q vary only weakly on the typical length scale. This means that the soliton width should be significantly larger than the lattice spacing $a = 1$, e.g. $\Gamma > 10$. Thus, continuum and semiclassical approximations work well in a consistent area of the soliton parameters.

(ii) Next we consider a ferromagnetic Heisenberg chain with a biaxial local anisotropy:

$$\mathcal{H}_2 = -J \sum_n \left[\hat{\mathbf{S}}_n \cdot \hat{\mathbf{S}}_{n+1} + \tau_x \hat{S}_n^x \hat{S}_n^x + \tau_z \hat{S}_n^z \hat{S}_n^z \right]. \tag{26}$$

The square variance of the energy is given by

$$\langle \mathcal{H}_2^2 \rangle - \langle \mathcal{H}_2 \rangle^2 = (\hbar S)^4 J^2 \sum_n \Bigg[\frac{1}{2S} \Big(\mathbf{s}_n \times (\mathbf{s}_{n-1} + \mathbf{s}_{n+1}) $$

$$+ 2 \left(1 - \frac{1}{2S} \right) [\tau_x (\mathbf{s}_n \times \mathbf{e}^x)(\mathbf{s}_n \cdot \mathbf{e}^x) + \tau_z (\mathbf{s}_n \times \mathbf{e}^z)(\mathbf{s}_n \cdot \mathbf{e}^z)] \Big)^2 $$

$$+ \frac{1}{8S^2} \Big((1 - \mathbf{s}_n \mathbf{s}_{n-1})^2 + (1 - \mathbf{s}_n \mathbf{s}_{n+1})^2 + 2 \left(1 - \frac{1}{2S} \right) [\tau_x^2 (\mathbf{s}_n \times \mathbf{e}^x)^4 $$

$$+ \tau_z^2 (\mathbf{s}_n \times \mathbf{e}^z)^4 + 2\tau_x \tau_z ((\mathbf{s}_n \cdot \mathbf{e}^x)(\mathbf{s}_n \cdot \mathbf{e}^z) - [\mathbf{s}_n \cdot (\mathbf{e}^x \times \mathbf{e}^z)]^2)] \Big) \Bigg]. \tag{27}$$

Proceeding as above, one can derive the following solutions of the continuum model (see, e.g., Kosevich *et al* 1990):

$$p(\xi, t) = \text{sgn}(v) \tanh \left(\frac{\xi - vt + \xi_0}{\Gamma} \right) \qquad q(\xi, t) = q_0 \tag{28}$$

with

$$\Gamma = \frac{1}{\sqrt{2(1 - 1/2S)(\tau_z - \tau_x \cos^2 q_0)}} \qquad v^2 = \frac{(\tau_x \sin(2q_0))^2 (1 - 1/2S)}{2(\tau_z - \tau_x \cos^2 q_0)} \tag{29}$$

where ξ_0, q_0 are constants and $\tau_z - \tau_x \cos^2 q_0 > 0$. Equations (28) describe moving kink solitons parametrized by q_0 with energy $E = 2/\Gamma$ above the ground state. For finite τ_x the velocity v vanishes for $q_0 \in \{0, \pi/2\}$ and takes its maximum value $v_{\text{max}}^2 = |\tau_x \cos(2q^*)|$ at $q_0 = q^*$ with

$$\cos(2q^*) = 2\frac{\tau_z}{\tau_x} - 1 - \text{sgn}\left(\frac{\tau_z}{\tau_x}\right) \sqrt{\left(2\frac{\tau_z}{\tau_x} - 1\right)^2 - 1}. \tag{30}$$

Inserting equations (28) into the continuum version of (27) leads to a divergence in Ω_2 arising from the term proportional to τ_x^2. This contribution is almost uniform over the whole system except for an area around the centre of the kink. Moreover, the same divergence occurs if we evaluate Ω_2 for the classical ground state of the model (26). The explanation for this behaviour is that, unlike in the previous model, the quantum mechanical ground state of (26) is not described exactly by our *ansatz* (7). Thus, the divergent contribution of order $1/S^2$ is clearly an artifact of our variational approach due to a more complicated structure of the quantum mechanical ground state, which does not correspond trivially to the classical ground-state solution. Note that a similar infinite term in Ω_2 arises for the classical ground state of an antiferromagnetic Heisenberg model—e.g. (12) with $J < 0$.

Here the divergence in order $1/S^2$ is due to the contribution from the isotropic exchange in the Hamiltonian.

Since we are interested in physically valid quantum fluctuations in time-dependent excitations within a semiclassical approach, we renormalize $\langle\mathcal{H}_2^2\rangle - \langle\mathcal{H}_2\rangle^2$ by neglecting Ω_2. The remaining contribution is calculated easily, giving

$$\Omega_1 = \frac{1}{S}\frac{v^2}{\Gamma} = \frac{1}{S}\frac{(\tau_x \sin(2q_0))^2(1-1/2S)^{3/2}}{(2(\tau_z - \tau_x \cos^2 q_0))^{1/2}}. \tag{31}$$

This leading order of the energy variance vanishes of course in the static case $q_0 \in \{0, \pi/2\}$ and takes its maximum at $q_0 = q^{**}$ where

$$\cos(2q^{**}) = 2\left(2\frac{\tau_z}{\tau_x} - 1\right) - 2\,\mathrm{sgn}\left(\frac{\tau_z}{\tau_x}\right)\sqrt{\left(2\frac{\tau_z}{\tau_x} - 1\right)^2 - \frac{3}{4}}. \tag{32}$$

Obviously, q^* and q^{**} are not the same.

In the case where $\tau_x = 0$, the kink solitons become static, and the exact quantum ground state is again the trivial ferromagnetic state. Thus, $\Omega_1 = 0$ and no unphysical divergency arises in Ω_2:

$$\Omega_2 = \frac{1}{S^2}\frac{1}{3\sqrt{2}}\sqrt{\left(1 - \frac{1}{2S}\right)}\tau_z^{3/2}\left(1 + 4\left(1 - \frac{1}{2S}\right)\right). \tag{33}$$

Comparing $\sqrt{\Omega_2}$ with the energy of the kink excitation, we again conclude that the semiclassical description should be valid for solitons with large width and low energy.

(iii) The isotropic Heisenberg ferromagnet on a two-dimensional infinite square lattice is given by

$$\mathcal{H}_3 = -J\sum_{m,n}\hat{\boldsymbol{S}}_{m,n}\cdot(\hat{\boldsymbol{S}}_{m+1,n} + \hat{\boldsymbol{S}}_{m,n+1}). \tag{34}$$

In appropriate units we find in the continuum approximation

$$\langle\mathcal{H}_3\rangle = \frac{1}{2}\int \mathrm{d}^2x\left(\frac{(\boldsymbol{\nabla}p)^2}{1-p^2} + (1-p^2)(\boldsymbol{\nabla}q)^2\right). \tag{35}$$

Equation (35) defines a two-dimensional conformally invariant field theory that has been investigated by Belavin and Polyakov (1975). The fields p, q parametrize points on the unit sphere S^2. Compactifying the two-dimensional plane by an infinite point we can consider the solutions of the Hamiltonian (35) as $S^2 \to S^2$ mappings. These mappings can be classified in homotopical classes characterized by the degree of mapping d with

$$|d| = \frac{1}{8\pi}\int \mathrm{d}^2x\,\varepsilon_{\alpha\beta\gamma}\varepsilon_{\mu\nu}s^\alpha\frac{\partial s^\beta}{\partial x_\mu}\frac{\partial s^\gamma}{\partial x_\nu} = \frac{1}{4\pi}\int \mathrm{d}\varphi(\boldsymbol{x})\,\mathrm{d}(\cos\vartheta(\boldsymbol{x})) \tag{36}$$

which is the number of times that the sphere is covered in the course of the mapping. As shown by the above authors,

$$\langle\mathcal{H}_3\rangle = 4\int \mathrm{d}^2z\,\frac{1}{(1+|w|^2)^2}\left(\frac{\partial w}{\partial z}\frac{\partial \bar{w}}{\partial \bar{z}} + \frac{\partial \bar{w}}{\partial z}\frac{\partial w}{\partial \bar{z}}\right) \geqslant 4\pi|d| \tag{37}$$

holds with $w(z, \bar{z}) = \cot(\vartheta/2)\mathrm{e}^{\mathrm{i}\varphi}$ and $z = x_1 + \mathrm{i}x_2$. The minimum in (37) is realized by instanton solutions that are given by arbitrary meromorphic functions $w(z)$:

$$w(z) = \prod_i\left(\frac{z - a_i}{R}\right)^{m_i}\prod_i\left(\frac{R}{z - b_i}\right)^{n_i} \tag{38}$$

with $m_i, n_i > 0$ and $a_i \neq b_j$ for all i, j and the degree given by $d = \max\{\sum_i m_i, \sum_i n_i\}$. The real scale parameter R does not influence the energy of these static excitations due to the conformal invariance of the model.

Let us now consider a single instanton simply given by $w = (z/R)^\nu$, $d = |\nu|$, or

$$p = \frac{|z|^{2\nu} - R^{2\nu}}{|z|^{2\nu} + R^{2\nu}} \qquad q = \nu \arg(z). \tag{39}$$

Clearly we have $\Omega_1 = 0$, and for Ω_2 one obtains

$$\Omega_2 = \frac{1}{S^2 R^2} \frac{2\pi^2}{3} \frac{\nu^2 - 1}{\sin(\pi/|\nu|)} \qquad |\nu| > 1 \tag{40}$$

and

$$\Omega_2 = \frac{1}{S^2 R^2} \frac{4\pi}{3} \qquad |\nu| = 1. $$

In contrast to the energy of the continuum model, this quantity is not independent of R, but scales with $1/R^2$. Again, for the semiclassical description to be valid, $\sqrt{\Omega_2}$ should be small compared with the energy $\langle \mathcal{H}_3 \rangle = 4\pi d$. This can be achieved for arbitrarily high energies provided that the width of the instanton is sufficiently large.

Next we consider a solution consisting of two instantons separated by distance $2l$,

$$w(z) = \left(\frac{z-l}{R}\right)^\mu \left(\frac{z+l}{R}\right)^\nu \tag{41}$$

and find

$$\Omega_2 = \frac{1}{2S^2} \int d^2z \left(\frac{|\partial w/\partial z|^2}{(1+|w|^2)^2}\right)^2 = \frac{1}{2S^2 R^2} F\left(\mu, \nu; \frac{l}{R}\right) \tag{42}$$

with

$$F(\mu, \nu; a) = \int d^2z \left(\frac{|z-a|^{\mu-1}|z+a|^{\nu-1}((\mu+\nu)z + (\mu-\nu)a)}{1 + |z-a|^{2\mu}|z+a|^{2\nu}}\right)^4. \tag{43}$$

Again, the square variance of the energy scales with $1/R^2$. Unfortunately, the quantity $F(\mu, \nu; a)$ cannot be expressed in terms of elementary functions; e.g. in the case where $\mu = \nu$, one obtains after some algebra

$$F(\mu, \mu; a) = a^{-8\mu-2} \int d^2x \frac{|\boldsymbol{x}|^{4\mu-4}|\boldsymbol{x}+\boldsymbol{e}|}{(a^{-4\mu} + |\boldsymbol{x}|^{2\mu})^4} \tag{44}$$

with $\boldsymbol{e}$ being an arbitrary unit vector.

(iv) Finally we consider an anisotropic two-dimensional Heisenberg Hamiltonian:

$$\mathcal{H}_4 = -J \sum_{m,n} \left[\hat{\boldsymbol{S}}_{m,n} \cdot (\hat{\boldsymbol{S}}_{m+1,n} + \hat{\boldsymbol{S}}_{m,n+1}) - \lambda \hat{S}^z_{m,n} \hat{S}^z_{m,n} \right]. \tag{45}$$

Choosing $\lambda > 0$ and the lattice lying in the x–y-plane, the classical ground state is given by a parallel spin configuration in this easy plane. Furthermore, we have

$$\langle \mathcal{H}_4^2 \rangle - \langle \mathcal{H}_4 \rangle^2 = (\hbar S)^4 J^2 \sum_{m,n} \left[\frac{1}{2S} \left(\boldsymbol{s}_{m,n} \times (\boldsymbol{s}_{m-1,n} + \boldsymbol{s}_{m+1,n} + \boldsymbol{s}_{m,n-1} + \boldsymbol{s}_{m,n+1}) \right. \right.$$

$$\left. - 2\left(1 - \frac{1}{2S}\right) \lambda (\boldsymbol{s}_{m,n} \cdot \boldsymbol{e}^z)(\boldsymbol{s}_{m,n} \times \boldsymbol{e}^z) \right)^2$$

$$+ \frac{1}{8S^2} \left((1 - \boldsymbol{s}_{m,n} \cdot \boldsymbol{s}_{m-1,n})^2 + (1 - \boldsymbol{s}_{m,n} \cdot \boldsymbol{s}_{m+1,n})^2 \right.$$

$$+ (1 - \boldsymbol{s}_{m,n} \cdot \boldsymbol{s}_{m,n-1})^2 + (1 - \boldsymbol{s}_{m,n} \cdot \boldsymbol{s}_{m,n+1})^2$$

$$+ 2\left(1 - \frac{1}{2S}\right)\lambda^2 (\boldsymbol{s}_{m,n} \times \boldsymbol{e}^z)^4\bigg)\bigg]. \tag{46}$$

For sufficiently large λ, planar vortices are stable excitations (Gouvea *et al* 1989). These objects are given in a continuum approximation by

$$p(\boldsymbol{x}, t) = 0 \qquad q(\boldsymbol{x}, t) = \nu \tan^{-1}\left(\frac{x_2}{x_1}\right) \tag{47}$$

with energy $E = \pi \nu^2 \ln(L/a)$, where we have chosen appropriate units as before. The integer ν is called the vorticity, L is the size of the system and $a = 1$ is the lattice spacing, which is a lower cut-off for the integration. The energy diverges logarithmically with the system size, due to the fact that the spin configuration is not parallel far away from the vortex centre. In this sense, the planar vortex is not localized.

Inserting such a static planar solution into (46) obviously gives $\Omega_1 = 0$ and in Ω_2 a contribution proportional to λ^2 that diverges quadratically with growing L. This effect is completely analogous to the divergence in the model (26) and is caused by the inexact description of the quantum ground state within our variational *ansatz*. So we renormalize Ω_2 by neglecting this artificial term, which is identical for any planar solution and therefore, in particular, not sensitive to the vortex (47). The remaining expression for the quantum mechanical variance of the energy is

$$\Delta E = \frac{1}{2S}\sqrt{\frac{\pi}{6}}\nu^2\sqrt{1 - \frac{1}{L^2}}. \tag{48}$$

In a classical easy-plane model of the above type, a topological phase transition, or Kosterlitz–Thouless transition, occurs at a certain temperature T_{KT} (Kosterlitz and Thouless 1973, Kosterlitz 1974). Below this temperature, vortices and antivortices (differing in the sign of the topological charge ν) are bound in pairs, while they become mobile above T_{KT}.

Now we use our result (48) to estimate quantum corrections to the value of the critical temperature T_{KT}. We assume that only vortices with $|\nu| = 1$ are present in our system and follow some rough approximations in the references given.

In the free energy $F = E - TS$, the quantum fluctuations will give an additional contribution to the entropy S. For a single vortex the classical entropy is $S = \ln(L^2)$, since the vortex can be placed anywhere in the system. In our semiclassical description we have to take into account the uncertainty of the energy:

$$S = \ln\left(L^2\left(1 + \frac{\Delta E}{E}\right)\right) = 2\ln L + \frac{\Delta E}{E} + \mathrm{O}\left(\frac{1}{S^2}\right). \tag{49}$$

The entropy term will dominate in the free energy above a temperature

$$T = \frac{\pi}{2}\frac{1}{1 + \Delta E/[2\pi(\ln L)^2]} = \frac{\pi}{2}\left(1 - \frac{\Delta E}{2\pi(\ln L)^2}\right) + \mathrm{O}\left(\frac{1}{S^2}\right) \tag{50}$$

which reduces to the classical estimate $T_{KT} = \pi/2$ for $L \to \infty$. Thus, we conclude that in an infinite system there is no quantum correction to the Kosterlitz–Thouless temperature of first order in $1/S$, but a logarithmic finite-size contribution arises in this order.

5. Conclusions

In this work we investigate a large family of spin models in the semiclassical regime with respect to quantum fluctuations. Our main result is given by equations (10) and (11)

which provide a physically relevant expression for the quantum fluctuations of the energy in low orders in $1/S$. In particular, the contribution in first order is purely due to the time dependence of the spin configuration in the semiclassical description. For a static spin configuration the square variance of the energy is of order $1/S^2$. The term of first order is a natural property of a state vector with a non-trivial time dependence, which is consequently not an eigenstate of the Hamiltonian. The terms of higher order can often be used as a criterion for the validity of the semiclassical approach.

These findings are valid for a large variety of spin models in arbitrary dimensions. In the previous section we have illustrated this for several important spin models.

Acknowledgment

Appendix A. Expectation values within coherent states

Let $\mathcal{P}[\hat{S}^+, \hat{S}^-, \hat{S}^z]$ be an arbitrary product of operator-valued spin components. With U given in equation (3) we have

$$\langle S; \vartheta, \varphi | \mathcal{P}[\hat{S}^+, \hat{S}^-, \hat{S}^z] | S; \vartheta, \varphi \rangle = \langle S | \mathcal{P}[U^+ \hat{S}^+ U, U^+ \hat{S}^- U, U^+ \hat{S}^z U] | S \rangle. \tag{A1}$$

The following equalities hold:

$$U^+ \hat{S}^+ U = e^{i\varphi} \left(\cos^2\left(\frac{\vartheta}{2}\right) \hat{S}^+ - \sin^2\left(\frac{\vartheta}{2}\right) \hat{S}^- + \sin\vartheta \, \hat{S}^z \right) \tag{A2}$$

$$U^+ \hat{S}^z U = -\frac{1}{2} \sin\vartheta \, \hat{S}^+ - \frac{1}{2} \sin\vartheta \, \hat{S}^- + \cos\vartheta \, \hat{S}^z. \tag{A3}$$

Applying $\hat{S}^+$, $\hat{S}^-$ to states of the type $|S - m\rangle$ gives a contribution of leading order $\sqrt{S}$, while $\hat{S}^z$ gives a factor of leading order S. From such arguments it is easily seen that the leading term in equation (A1) is proportional to the product of the classical spin components given by $s_{\vartheta,\varphi}$:

$$\lim_{\substack{S \to \infty \\ \hbar S = S^{cl} = \text{constant}}} \langle S; \vartheta, \varphi | \mathcal{P}[\hat{S}^+, \hat{S}^-, \hat{S}^z] | S; \vartheta, \varphi \rangle = \mathcal{P}[S^{cl} s^+_{\vartheta,\varphi}, S^{cl} s^-_{\vartheta,\varphi}, S^{cl} s^z_{\vartheta,\varphi}] \tag{A4}$$

where $\hbar S = S^{cl} = $ constant is the classical spin length. In the classical limit taken above, all terms of higher order in $1/S$ (or equivalently in $\hbar$) drop out. Of course, the details of these quantum contributions depend on the structure of $\mathcal{P}[\hat{S}^+, \hat{S}^-, \hat{S}^z]$, i.e. the ordering of the spin operators.

Using equations (A2) and (A3) expectation values of type (A1) can be calculated easily. Here we give a list of diagonal elements useful for the derivation of equation (10):

$$\langle S; \vartheta, \varphi | \hat{S}^z \hat{S}^z | S; \vartheta, \varphi \rangle = (\hbar S)^2 \left(\cos^2\vartheta + \frac{1}{2S} \sin^2\vartheta \right) \tag{A5}$$

$$\langle S; \vartheta, \varphi | \hat{S}^+ \hat{S}^- + \hat{S}^- \hat{S}^+ | S; \vartheta, \varphi \rangle = 2(\hbar S)^2 \left(\sin^2\vartheta + \frac{1}{S}\left(1 + \cos^2\vartheta\right) \right) \tag{A6}$$

$$\langle S; \vartheta, \varphi | \hat{S}^+ \hat{S}^z + \hat{S}^z \hat{S}^+ | S; \vartheta, \varphi \rangle = 2(\hbar S)^2 \left(1 - \frac{1}{2S} \right) e^{i\varphi} \cos\vartheta \sin\vartheta \tag{A7}$$

$$\langle S; \vartheta, \varphi | \hat{S}^z \hat{S}^z \hat{S}^z | S; \vartheta, \varphi \rangle = (\hbar S)^3 \left(\cos^3\vartheta + \left(\frac{3}{2S} - \frac{1}{2S^2}\right) \cos\vartheta \sin^2\vartheta \right) \tag{A8}$$

$$\langle S; \vartheta, \varphi | \hat{S}^+ \hat{S}^z \hat{S}^+ | S; \vartheta, \varphi \rangle = (\hbar S)^3 \left(1 - \frac{1}{2S}\right)\left(1 - \frac{1}{S}\right) e^{i2\varphi} \cos \vartheta \sin^2 \vartheta \tag{A9}$$

$$\langle S; \vartheta, \varphi | \hat{S}^z \hat{S}^+ \hat{S}^z | S; \vartheta, \varphi \rangle = (\hbar S)^3 \left(1 - \frac{1}{S}\right) e^{i\varphi} \left(\cos^2 \vartheta \sin \vartheta + \frac{1}{2S} \sin^3 \vartheta\right) \tag{A10}$$

$$\langle S; \vartheta, \varphi | \hat{S}^+ \hat{S}^z \hat{S}^z + \hat{S}^z \hat{S}^z \hat{S}^+ | S; \vartheta, \varphi \rangle$$
$$= 2(\hbar S)^3 e^{i\varphi} \left(\left(1 - \frac{1}{2S}\right)\left(1 - \frac{1}{S}\right) \cos^2 \vartheta \sin \vartheta + \frac{1}{2S} \sin \vartheta\right) \tag{A11}$$

$$\langle S; \vartheta, \varphi | \hat{S}^z \hat{S}^z \hat{S}^z \hat{S}^z | S; \vartheta, \varphi \rangle$$
$$= (\hbar S)^4 \left(\cos^4 \vartheta + \left(\frac{3}{S} - \frac{5}{2S^2} + \frac{5}{8S^3}\right) \cos^2 \vartheta \sin^2 \vartheta + \left(\frac{1}{2S^2} + \frac{1}{8S^3}\right) \sin^2 \vartheta\right) \tag{A12}$$

$$\langle S; \vartheta, \varphi | \hat{S}^z \hat{S}^z (\hat{S}^+ \hat{S}^- + \hat{S}^- \hat{S}^+) + (\hat{S}^+ \hat{S}^- + \hat{S}^- \hat{S}^+) \hat{S}^z \hat{S}^z | S; \vartheta, \varphi \rangle$$
$$= 2(\hbar S)^4 \left(\left(2 - \frac{6}{S} + \frac{5}{S^2} - \frac{5}{4S^3}\right) \cos^2 \vartheta \sin^2 \vartheta + \frac{2}{S} \cos^2 \vartheta\right.$$
$$\left. + \left(\frac{1}{S} + \frac{1}{4S^3}\right) \sin^2 \vartheta\right) \tag{A13}$$

$$\langle S; \vartheta, \varphi | \hat{S}^z \hat{S}^z (\hat{S}^+ \hat{S}^+ + \hat{S}^- \hat{S}^-) + (\hat{S}^+ \hat{S}^+ + \hat{S}^- \hat{S}^-) \hat{S}^z \hat{S}^z | S; \vartheta, \varphi \rangle$$
$$= 2(\hbar S)^4 \cos(2\varphi) \left(\left(2 - \frac{6}{S} + \frac{5}{S^2} - \frac{5}{4S^3}\right) \cos^2 \vartheta \sin^2 \vartheta\right.$$
$$\left. + \left(\frac{1}{S} - \frac{1}{4S^3}\right) \sin^2 \vartheta\right). \tag{A14}$$

Appendix B. Coherent states and the classical limits of spin systems

Let us consider a system of spins $\{\boldsymbol{S}_i\}_{i \in I}$. The dynamics is given by a quantum Hamiltonian $\mathcal{H}[\{\hat{\boldsymbol{S}}_i\}_{i \in I}]$, which is taken to be an arbitrary polynomial in the spin components.

We now evaluate the Heisenberg equation of motion for the ith spin at a chosen time $t = t_0$ in terms of a tensor product of spin-coherent states:

$$|\psi(t_0)\rangle = \bigotimes_{i \in I} |S_i; \vartheta_i, \varphi_i\rangle \tag{B1}$$

and denote by $\langle \ \rangle$ an expectation value in the state (B1):

$$\left(\frac{d}{dt} \langle \hat{\boldsymbol{S}}_i \rangle\right)_{t=t_0} = \frac{1}{i\hbar} (\langle [\hat{\boldsymbol{S}}_i, \mathcal{H}] \rangle)_{t=t_0}. \tag{B2}$$

The right-hand side of this equation can be evaluated straightforwardly in terms of the variables ϑ_i, φ_i, while for the left-hand side we need information about the time evolution of the wave function $|\psi(t)\rangle$.

The time evolution of the spin expectation values is

$$\langle \psi(t) | \hat{\boldsymbol{S}}_i | \psi(t) \rangle = \langle \psi(t_0) | \exp\left(+\frac{i}{\hbar} \mathcal{H}(t - t_0)\right) \hat{\boldsymbol{S}}_i \exp\left(-\frac{i}{\hbar} \mathcal{H}(t - t_0)\right) | \psi(t_0) \rangle$$
$$= \langle \hat{\boldsymbol{S}}_i \rangle_{t_0} + \frac{i(t - t_0)}{\hbar} \langle [\mathcal{H}, \hat{\boldsymbol{S}}_i] \rangle_{t_0} + \frac{1}{2} \left(\frac{i(t - t_0)}{\hbar}\right)^2 \langle [\mathcal{H}, [\mathcal{H}, \hat{\boldsymbol{S}}_i]] \rangle_{t_0} + \cdots. \tag{B3}$$

The diagonal elements in the expansion (B3) are products of expressions of the form (A1) and therefore reduce in the limit $S \to \infty$, $\hbar \to 0$, $\hbar S = $ constant to the classical values.

For example, for the first commutator we have

$$\lim_{\substack{S_j \to \infty \\ \hbar S_j = S_j^{cl} = \text{constant} \\ j \in I}} \frac{\mathrm{i}}{\hbar} \langle [\mathcal{H}, \hat{\boldsymbol{S}}_i] \rangle_{t_0} = -S_i^{cl} \boldsymbol{s}_i \times \frac{\partial \mathcal{H}[\{S_j^{cl} \boldsymbol{s}_j\}_{j \in I}]}{\partial (S_i^{cl} \boldsymbol{s}_i)} \tag{B4}$$

with $\boldsymbol{s}_i = (\sin \vartheta_i \cos \varphi_i, \sin \vartheta_i \sin \varphi_i, \cos \vartheta_i)$. The right-hand side of this equation is simply the classical Poisson bracket $\{S_i^{cl} \boldsymbol{s}_i, \mathcal{H}\}$ occurring in the well-known Landau–Lifshitz equation, i.e. the equation of motion for a classical spin system. Similar arguments hold for the higher commutators in (B3), and we end up with

$$\lim_{\substack{S_j \to \infty \\ \hbar S_j = S_j^{cl} = \text{constant} \\ j \in I}} \langle \psi(t) | \hat{\boldsymbol{S}}_i | \psi(t) \rangle = S_i^{cl} \boldsymbol{s}_i + (t - t_0)\{S_i^{cl} \boldsymbol{s}_i, \mathcal{H}\} + \frac{(t - t_0)^2}{2} \{\{S_i^{cl} \boldsymbol{s}_i, \mathcal{H}\}, \mathcal{H}\} + \cdots.$$

$$\tag{B5}$$

Thus, we have confirmed that the classical limit of the quantum mechanical time evolution (B3) reproduces the motion of a classical spin vector in the case of an arbitrary Hamiltonian.

By similar considerations, one can convince oneself that minimizing the action

$$\mathcal{S} = \int_{t_1}^{t_2} \mathrm{d}t \, \langle \psi(t) | \mathrm{i} \hbar \, \frac{\mathrm{d}}{\mathrm{d}t} - \mathcal{H} | \psi(t) \rangle \tag{B6}$$

in the classical limit with respect to the functions $\vartheta_i(t)$, $\varphi_i(t)$ also leads to the classical equations. This should be expected since the variational principle concerning (B6) (with arbitrary wave function $|\psi(t)\rangle$) is equivalent to the Heisenberg equation of motion.

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