A long-wave action of spin Hamiltonians and the inverse problem of the calculus of variations.

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(Dated: December 7, 2018)

We suggest a method of derivation of the long-wave action of the model spin Hamiltonians using the non-linear partial differential equations of motions of the individual spins. According to the Vainberg’s theorem the set of these equations are (formal) potential if the symmetry analysis for the Frechet derivatives of the system is true. The case of Heisenberg (anti)ferromagnets is considered. It is shown the functional whose stationary points are described by the equations coincides with the long-wave action and includes the non-trivial topological term (Berry phase).
The most of rigorous results in the dynamics of a one- or two-dimensional isotropic Heisenberg antiferromagnet due to a presence of non-trivial topological term in the action (Berry phase) has been obtained in a coherent state path integral formulation. This approach starts with the derivation a path integral representation for the partition function of an individual spin \( Z = \text{Tr} \exp(-\beta H(S)) \) where the Hamiltonian \( H(S) \) is a linear function of the spin operator \( S \). Further, this result is generalized for a lattice problem using the fact the Hilbert space of the many spin system is the direct product of the one-spin Hilbert spaces at each site. In path-integral formulation is convenient to use an overcomplete basis of spin coherent states \( |\vec{N}\rangle \) labeled by the points \( \vec{N} \) on the surface of the unit sphere with the expectation value of the spin \( \langle \vec{N}|\vec{S}|\vec{N}\rangle = S\vec{N} \). The exponential in the expression for \( Z \) is written as the Trotter product of a large number of exponentials each evolving the system over an infinitesimal imaginary time interval \( \Delta \tau \) and using the resolution of unity \( 1 = \int \frac{d\vec{N}}{2\pi} |\vec{N}\rangle\langle\vec{N}| \) between the intervals (the integral is over the unit sphere). This procedure leads to the following representation for the partition function

\[
Z = \int D\vec{N}(\tau) \exp \left[ \int_0^\beta d\tau \left( \langle \vec{N}(\tau) | \frac{d}{d\tau} | \vec{N}(\tau) \rangle - H(S\vec{N}(\tau)) \right) \right],
\]

where \( H(S\vec{N}(\tau)) \) is the Hamiltonian in spin coherent representation. The first term in the action is the Berry phase term \( S_B \) and represents the overlap between the coherent states at two infinitesimally separated times. The manipulation \( S_B \) into a physically more transparent form may be found, for example, in Ref.\(^2\). The result is

\[
S_B = iS \int_0^\beta d\tau \int_0^1 du \left( \vec{N} \left[ \frac{\partial \vec{N}}{\partial u} \times \frac{\partial \vec{N}}{\partial \tau} \right] \right),
\]

where \( u \) is a dummy integration variable, \( |\vec{N}(\tau, u)\rangle \) is defined by

\[
|\vec{N}(\tau, u)\rangle = \exp \left( u \left( z(\tau)\hat{S}^+ - z^*(\tau)\hat{S}^- \right) \right) |\vec{N} = (0, 0, 1)\rangle,
\]

with the properties \( |\vec{N}(\tau, u = 1)\rangle = |\vec{N}(\tau)\rangle \), \( |\vec{N}(\tau, u = 0)\rangle = |\vec{N} = (0, 0, 1)\rangle \) and the complex number \( z \) is given in spherical coordinates \( z = -\frac{\phi}{2} \exp(-i\phi) \). The \( S_B \) presents the oriented area contained within the closed loop defined by \( \vec{N}(\tau), 0 \leq \tau \leq \beta, \vec{N}(0) = \vec{N}(\beta) \) on the spin sphere.

In this Letter, it will be demonstrated how the long-wave action for spin Hamiltonians can be derived by using the non-linear differential equations of motion of spins via the solving
of the inverse problem of the calculus of variations: that is, finding the functional whose stationary points are described by the descriptive equations.

As is well known the most fundamental question is whether the functional exists for a given operator. In Ref.\(^3\), Atherton and Homsy have suggested a stringent and elegant formalism based on Vainberg’s theorem\(^4\) to derive the operational formulas for the case of an arbitrary number of nonlinear differential equations in an arbitrary number of independent variables and of arbitrary order to determine whether given differential operators are potential.

As the simplest illustration of the method we consider the case of a Heisenberg ferromagnet with the spin Hamiltonian

\[
H = -\frac{1}{2} \sum_{(im)} J_{im} \vec{S}_i \cdot \vec{S}_m
\]

where the \(\vec{S}_i\) are spin \(S\) quantum spin operators on the \(i\)th sites of a \(n\)-dimensional hypercubic lattice. The exchange constant \(J_{im} > 0\) is non-zero just for the nearest neighbors. The non-linear differential equations describing the dynamics of Heisenberg ferromagnet can be obtained by taking the diagonal matrix elements of the equation of motion for the raising operator

\[
i \hbar \frac{\partial}{\partial t} |\Omega\rangle = \left[ S_i^+, H \right] |\Omega\rangle
\]

of the \(i\)th spin in spin-coherent representation \(|\Omega\rangle = \prod_{i=1}^{N} |\theta_i, \phi_i\rangle\), where \(0 \leq \theta_i \leq \pi\) and \(0 \leq \phi_i < 2\pi\) parametrize the spin states on the unit sphere\(^5\). In continuum approximation the coupled c-number equations for the real variables \(\theta\) and \(\phi\) depending on the time \(t \in [t_1, t_2]\) and space coordinates \(\vec{r} \in \mathbb{R}^n\) can be written as following (hereafter the lattice constant is unit)

\[
0 = -S \sin \Theta \frac{\partial \phi}{\partial t} + \frac{JS^2}{\hbar} \left( \Delta \Theta - \cos \Theta \sin \Theta \left( \nabla \phi \right)^2 \right),
\]

\[
0 = S \frac{\partial \Theta}{\partial t} + \frac{JS^2}{\hbar} \left( 2 \cos \Theta \left( \nabla \phi \nabla \Theta \right) + \sin \Theta \Delta \phi \right). \tag{4}
\]

These equations present a vector of differential operators \(R^j(z_k) = 0\) \((j, k = 1, 2\) and \(z_1 = \Theta, z_2 = \phi)\)

\[
R^1 = -S \sin \Theta \frac{\partial \phi}{\partial t} + \frac{JS^2}{\hbar} \left( \Delta \Theta - \cos \Theta \sin \Theta \left( \nabla \phi \right)^2 \right),
\]

\[
R^2 = S \sin \Theta \frac{\partial \Theta}{\partial t} + \frac{JS^2}{\hbar} \left( 2 \sin \Theta \cos \Theta \left( \nabla \phi \nabla \Theta \right) + \sin^2 \Theta \Delta \phi \right). \tag{5}
\]

The second equation in (4) is multiplied by the factor \(\sin \Theta\) that is necessary for the further symmetry analysis. The inverse problem is solved if an operator can be proven to be a potential operator, i.e. an analysis of the Frechet derivatives is symmetrical (Vainberg’s theorem). According to the procedure in Ref.\(^3\) we evaluate the "two-tensor" of Frechet derivatives
in the directions $u_k$

$$R^i_{1,k} = \lim_{\epsilon \to 0} \frac{1}{\epsilon} \left( R^i(z_k + \epsilon u_k) - R^i(z_k) \right),$$  \hspace{1cm} (6)

$$R^1_{1} = -u_1 S \cos \Theta \frac{\partial \phi}{\partial t} + \frac{JS^2}{h} \left( \Delta u_1 - u_1 \cos 2\Theta \left( \nabla \phi \right)^2 \right),$$  \hspace{1cm} (7)

$$R^1_{2} = -S \sin \Theta \frac{\partial u_2}{\partial t} - \frac{JS^2}{h} \sin 2\Theta \left( \nabla \phi \nabla u_2 \right),$$  \hspace{1cm} (8)

$$R^2_{1} = S \sin \Theta \frac{\partial u_1}{\partial t} + u_1 S \cos \Theta \frac{\partial \Theta}{\partial t}$$

$$+ \frac{JS^2}{h} \left( u_1 \sin 2\Theta \Delta \phi + \sin 2\Theta \left( \nabla u_1 \nabla \phi \right) + 2u_1 \cos 2\Theta \left( \nabla \phi \nabla \Theta \right) \right),$$  \hspace{1cm} (9)

$$R^2_{2} = \frac{JS^2}{h} \sin^2 \Theta \Delta u_2 + \frac{JS^2}{h} \sin 2\Theta \left( \nabla u_2 \nabla \Theta \right).$$  \hspace{1cm} (10)

The symmetry requirement is satisfied if \( \int \psi_j R^j_{1,k} u_k dV = \int u_j R^j_{1,k} \psi_j dV \) for every \( \psi_j, u_k \) in the range of the \( R^j \). The integral is taken over all space coordinates and time \( \int^t_{t_1} dV \equiv \int d\vec{r} \). The respective ordering of the vectors \( R^j \) and \( z_k \) is very important. It determines the form of the variational integral and required symmetry conditions. The symmetry test yields to the following boundary conditions

$$\int \psi_1 R^1_{1} u_1 dV = \int u_1 R^1_{1} \psi_1 dV \Rightarrow \oint_S (\psi_1 \nabla u_1 - u_1 \nabla \psi_1) d\vec{S} = 0,$$  \hspace{1cm} (11)

$$\int \psi_1 R^1_{2} u_2 dV = \int u_2 R^2_{1} \psi_1 dV \Rightarrow \oint_S \sin 2\Theta \psi_1 u_2 \nabla \phi d\vec{S} = 0, \psi_1 u_2 \sin \Theta|_{t_1}^{t_2} = 0,$$  \hspace{1cm} (12)

$$\int \psi_2 R^2_{2} u_2 dV = \int u_2 R^2_{2} \psi_2 dV \Rightarrow \oint_S \sin^2 \Theta (\psi_2 \nabla u_2 - u_2 \nabla \psi_2) d\vec{S} = 0.$$  \hspace{1cm} (13)

The variational principle for the differential system can be constructed via the formula \( \int dV \int^1_0 d\lambda \ z_i R^i(\lambda z_i) \) where \( \int^1_0 d\lambda \) represents integration over the scalar variable \( \lambda \). It results in the following

$$F_1 = \int dV \int^1_0 d\lambda \ \Theta R_1(\lambda \Theta) = \int dV \int^1_0 d\lambda (-S \sin (\lambda \Theta)) \frac{\partial (\lambda \Theta)}{\partial \lambda} \frac{\partial \phi}{\partial t}$$

$$- \frac{JS^2}{2h} \int dV \left( \sin^2 \Theta \left( \nabla \phi \right)^2 + \left( \nabla \Theta \right)^2 \right) + C_1(\phi),$$  \hspace{1cm} (14)

$$F_2 = \int dV \int^1_0 d\lambda \ \phi R_2(\lambda \phi) = \int dV \left( S \sin \Theta \frac{\partial \Theta}{\partial t} \phi - \frac{JS^2}{2h} \sin^2 \Theta \left( \nabla \phi \right)^2 \right) + C_2(\Theta).$$  \hspace{1cm} (15)
The $C_{1,2}$ are some functions which are determined by the condition $F_1 = F_2 = F(\Theta, \phi)$. The using of the standard parametrization

$$\vec{S}(\lambda) = S\vec{N}(\lambda), \quad \vec{N}(\lambda) = (\sin(\lambda\Theta) \cos(\phi), \sin(\lambda\Theta) \sin(\phi), \cos(\lambda\Theta)),$$

where $\vec{N}(1) = \vec{N}(t)$ is the physical field and $\vec{N}(0) = (0, 0, 1)$ is the north pole of the physical sphere yields to the Berry phase term in (14)

$$S_B = \int dV \int_0^1 d\lambda (-S \sin(\lambda\Theta)) \frac{\partial(\lambda\Theta)}{\partial \lambda} \frac{\partial \phi}{\partial t}$$

$$= -S \int d\vec{r} \int_0^{t_2} t_1 dt \int_0^1 d\lambda \left( \vec{N} \left[ \frac{\partial N}{\partial \lambda} \times \frac{\partial \vec{N}}{\partial t} \right] \right).$$

(17)

The comparison of Eqs. (14, 15) gives the condition $\phi(t_1) = \phi(t_2)$. In contrary to a path integral formulation the claim $\vec{N}(t_1) = \vec{N}(t_2)$ arises as a necessary condition of potentiality of the differential operator. The following surface integrals must be zero $S_1 = \oint_S \Theta \nabla \Theta$ and $S_2 = \oint_S \phi \sin^2 \Theta \nabla \phi$. The unifying of Eqs.(14, 15) using the divergence theorem gives the final form of the functional

$$F = S_B - \frac{1}{\hbar} \int d\vec{r} \int_0^{t_2} dt \langle \Omega | H | \Omega \rangle,$$

(18)

where the part

$$\langle \Omega | H | \Omega \rangle = -JS^2 \left( n - \frac{1}{2} \sin^2 \Theta \left( \vec{\nabla} \phi \right)^2 - \frac{1}{2} \left( \vec{\nabla} \Theta \right)^2 \right)$$

(19)

is the density of the energy of the system. The expression (18) presents the long-vawe action (Euclidean) if to replace $t \rightarrow i\tau$ ($\tau \in [0, 1/T]$) and multiply the functional by $-i$.

The same analysis can be made for a generic Heisenberg two-sublattice antiferromagnet ($J < 0$) with the non-linear differential equations forming a vector of differential operators

$$R_1 = -S \sin \Theta_1 \frac{\partial \phi_1}{\partial t} + \frac{JS^2}{\hbar} \cos \Theta_1 \sin \Theta_2 \cos(\phi_1 - \phi_2) \left( n - \left( \vec{\nabla} \Theta_2 \right)^2 - \left( \vec{\nabla} \phi_2 \right)^2 \right)$$

$$+ \frac{JS^2}{\hbar} \cos \Theta_1 \sin \Theta_2 \sin(\phi_1 - \phi_2) \Delta \phi_2 + \frac{JS^2}{\hbar} \cos \Theta_2 \cos(\phi_1 - \phi_2) \Delta \Theta_2$$

$$+ \frac{2JS^2}{\hbar} \cos \Theta_1 \cos \Theta_2 \sin(\phi_1 - \phi_2) \left( \vec{\nabla} \phi_2 \vec{\nabla} \Theta_2 \right) + \frac{JS^2}{\hbar} \sin \Theta_1 \sin \Theta_2 \Delta \Theta_2$$

$$- \frac{JS^2}{\hbar} \sin \Theta_1 \cos \Theta_2 \left( n - \left( \vec{\nabla} \Theta_2 \right)^2 \right) = 0,$$

(20)
$R_2$ is the analogous equation with substitution of the lower indexes $1 \leftrightarrow 2$,

$$
R_3 = S \sin \Theta_1 \frac{\partial \Theta_1}{\partial t} + \frac{JS^2}{\hbar} \sin \Theta_1 \sin \Theta_2 \sin(\phi_2 - \phi_1) \left(n - \left(\nabla \Theta_1\right)^2 - \left(\nabla \phi_2\right)^2\right)
+ \frac{JS^2}{\hbar} \sin \Theta_1 \cos \Theta_2 \sin(\phi_2 - \phi_1) \Delta \Theta_2 + \frac{JS^2}{\hbar} \sin \Theta_1 \sin \Theta_2 \cos(\phi_1 - \phi_2) \Delta \phi_2
+ \frac{2JS^2}{\hbar} \sin \Theta_1 \cos \Theta_2 \cos(\phi_1 - \phi_2) \left(\nabla \Theta_2 \nabla \phi_2\right) = 0
$$

(21)

and the same equation $R_4$ with $1 \leftrightarrow 2$. Here, one must suppose $z_1 = \Theta_1, z_2 = \Theta_2, z_3 = \phi_1, z_4 = \phi_2$ where the lower indexes in $\Theta$ and $\phi$ denote the sublattices. The symmetry test $\int u_1 R_3^1 u_3 dV = \int u_3 R_3^1 u_1 dV$ and $\int u_2 R_3^2 u_4 dV = \int u_4 R_3^2 u_2 dV$ gives the time boundary conditions $\sin \Theta_1(t_1) = \sin \Theta_1(t_2)$ and $\sin \Theta_2(t_1) = \sin \Theta_2(t_2)$, correspondingly. The rest symmetry conditions determine the surface integrals which must be zero if the differential operator is potential. The construction of the variational principle gives

$$
F_1 = \int dV \left[ \int \frac{1}{0} d\lambda \Theta_1 R_1(\lambda \Theta_1) - S \int dV \int \frac{1}{0} d\lambda \left(\nabla_1 \left[ \frac{\partial \nabla_1}{\partial \lambda} \times \frac{\partial \nabla_1}{\partial t}\right]\right)\right]
+ \frac{JS^2}{\hbar} \int dV \sin \Theta_1 \left(\sin \Theta_2 \cos(\phi_1 - \phi_2) \left(n - \left(\nabla \phi_2\right)^2 - \left(\nabla \Theta_2\right)^2\right)\right)
+ \cos \Theta_2 \cos(\phi_1 - \phi_2) \Delta \Theta_2 + \sin \Theta_2 \sin(\phi_1 - \phi_2) \Delta \phi_2
+ 2 \cos \Theta_2 \sin(\phi_1 - \phi_2) \left(\nabla \Theta_2 \cdot \nabla \phi_2\right)
+ \frac{JS^2}{\hbar} \int dV \cos \Theta_1 \left(\cos \Theta_2 \left(n - \left(\nabla \Theta_2\right)^2\right) - \sin \Theta_2 \Delta \Theta_2\right) + C_1(\phi_1, \Theta_2, \phi_2)
$$

(22)

and

$$
F_2 = \int dV \left[ \int \frac{1}{0} d\lambda \phi_1 R_3(\lambda \phi_1) - S \int dV \int \frac{1}{0} d\lambda \left(\nabla_1 \left[ \frac{\partial \nabla_1}{\partial \lambda} \times \frac{\partial \nabla_1}{\partial t}\right]\right)\right]
+ \frac{JS^2}{\hbar} \int dV \sin \Theta_1 \left(\sin \Theta_2 \cos(\phi_1 - \phi_2) \left(n - \left(\nabla \phi_2\right)^2 - \left(\nabla \Theta_2\right)^2\right)\right)
+ \cos \Theta_2 \cos(\phi_1 - \phi_2) \Delta \Theta_2 + \sin \Theta_2 \sin(\phi_1 - \phi_2) \Delta \phi_2
+ 2 \cos \Theta_2 \sin(\phi_1 - \phi_2) \left(\nabla \Theta_2 \cdot \nabla \phi_2\right) + C_2(\Theta_1, \Theta_2, \phi_2),
$$

(23)

where $C_{1,2}$ are some functions. The comparison of both forms yields to $F(\Theta_1, \phi_1) + C_3(\Theta_2, \phi_2) = F_1 = F_2$ if the following conditions are fulfilled

$$
C_1(\phi_1, \Theta_2, \phi_2) = C_3(\Theta_2, \phi_2),
$$

(24)
\[ C_2(\Theta_1, \Theta_2, \phi_2) = C_3(\Theta_2, \phi_2) \]
\[ + \frac{JS^2}{\hbar} \int dV \cos \Theta_1 \left( \cos \Theta_2 \left( n - (\vec{\nabla}\Theta_2)^2 \right) - \sin \Theta_2 \Delta \Theta_2 \right). \]  
\tag{25}

The similar expression may be obtained for \( F(\Theta_2, \phi_2) \). It equals to \( F(\Theta_1, \phi_1) \) if to replace \( 1 \leftrightarrow 2 \). The final form for the variational principle may be obtained via an integration by parts using the divergence theorem and the boundary conditions found at the symmetry analysis. The result is
\[ F = -S \sum_{i=1}^{2} \int d\vec{r} \int_{t_1}^{t_2} dt \int_{0}^{1} d\lambda \left( \vec{N}_i \left[ \frac{\partial \vec{N}_i}{\partial \lambda} \times \frac{\partial \vec{N}_i}{\partial t} \right] \right) - \frac{1}{\hbar} \int d\vec{r} \int_{t_1}^{t_2} dt \langle \Omega | H | \Omega \rangle. \]  
\tag{26}

As in the previous case the expression coincides with the action and includes the Berry phase terms from each sublattice. The density of the energy is given as following
\[ \langle \Omega | H | \Omega \rangle = JS^2 \left( -n \sin \Theta_1 \sin \Theta_2 \cos(\phi_1 - \phi_2) - n \cos \Theta_1 \cos \Theta_2 ight. \]
\[ + \cos \Theta_1 \cos \Theta_2 \cos(\phi_1 - \phi_2) \left( \vec{\nabla}\Theta_1 \vec{\nabla}\Theta_2 \right) \]
\[ - \sin \Theta_1 \cos \Theta_2 \sin(\phi_1 - \phi_2) \left( \vec{\nabla}\phi_1 \vec{\nabla}\Theta_2 \right) \]
\[ + \cos \Theta_1 \sin \Theta_2 \sin(\phi_1 - \phi_2) \left( \vec{\nabla}\Theta_1 \vec{\nabla}\phi_2 \right) \]
\[ + \sin \Theta_1 \sin \Theta_2 \cos(\phi_1 - \phi_2) \left( \vec{\nabla}\phi_1 \vec{\nabla}\phi_2 \right) \]
\[ + \sin \Theta_1 \sin \Theta_2 \left( \vec{\nabla}\Theta_1 \vec{\nabla}\Theta_2 \right) \].  
\tag{27}

In conclusion, the method of derivation of the long-wave action for spin Hamiltonians is suggested via the solving of the inverse problem of calculus variations. The case of a Heisenberg (anti)ferromagnet is considered.

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