Geometrical Interpretation of Momentum and Crystal Momentum of Classical and Quantum Ferromagnetic Heisenberg Chains

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A rotationally invariant translation-generating functional for the continuum model of a ferromagnetic chain is found, resolving a long-standing paradox. The condition of rotational invariance leads to a topological quantization in the continuum classical model that corresponds to spin quantization in the equivalent discrete quantum model. The relation between the classical continuum model and the discrete quantum models is made precise.

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The classical continuum model of a one-dimensional Heisenberg ferromagnet[1] is an integrable nonlinear model exhibiting soliton solutions. As a continuum model that is invariant under continuous translations, it would normally be expected to have a well defined momentum functional that is the generator of translations, and is a constant of the motion. Such a function should also be fully rotationally invariant, but a long-standing paradox has been that a functional satisfying these criteria has not been found. In this Letter, I resolve this paradox and report that the "momentum" of this model is not a valid construction, but that a discrete (topologically quantized) set of well defined classical functionals analogous to the translation operator of a discrete quantum spin chain exist. The topological quantization of these classical functionals is analogous to the quantization of the discrete spins in the quantum models.

The continuum model describes a classical spin-density field $\mathbf{s}(x)$ with spin-length–conserving dynamics generated by the Poisson bracket algebra $\{s^i(x), s^j(x')\} = \epsilon^{ijk}s^k(x)\delta(x-x')$; the spin-density field obeys the conserved constraint $|\mathbf{s}(x)| = s_0$, where s_0 has dimensions action/length. The equation of motion is $\partial_t \mathbf{s}(x) = \{\mathbf{s}(x), H\}$, where $H = \int dx\, H(x)$ and $H = \frac{1}{2}j|\partial_x \mathbf{s}|^2$; from this, $\mathbf{s}\cdot\partial_t\mathbf{s}\times\partial_x\mathbf{s} = s_0^2\,\partial_x H$.

Since a momentum functional P must rescale as $P \to \lambda^{-1}P$ if $x \to \lambda x$, it must have the general form

$$P = \int \mathbf{A}(\mathbf{s}(x))\cdot\partial_x\mathbf{s}(x)\,dx, \tag{1}$$

where $\mathbf{A}(\mathbf{s})$ is a vector function of the spin field. From the Poisson bracket algebra and the equation of motion, we have

$$\{P, \mathbf{s}(x)\} = \partial_x\mathbf{s}(x) + f\Big(\mathbf{A}(\mathbf{s}(x))\Big)\partial_x\mathbf{s}(x), \tag{2}$$

$$\partial_t P = \int dx\, f(\mathbf{A}(\mathbf{s}))(\mathbf{s}\cdot\partial_t\mathbf{s}\times\partial_x\mathbf{s}), \tag{3}$$

where

$$f(\mathbf{A}(\mathbf{s})) = \mathbf{s}\cdot\frac{\partial}{\partial\mathbf{s}}\times\mathbf{A}(\mathbf{s}) - 1. \tag{4}$$

Equation (1) defines a true momentum functional *only* if $\mathbf{A}(\mathbf{s})$ satisfies the condition $f(\mathbf{A}(\mathbf{s})) = 0$.

This condition may be recognized as requiring $\mathbf{A}$ to be equivalent to the vector potential of a Dirac magnetic monopole,[2] and strictly has *no* solution; thus a true momentum functional does *not* exist! In the literature,[1] the commonly used expression for P is (1) with $\mathbf{A}(\mathbf{s})$ given by

$$\mathbf{A}(s) = \hat{\mathbf{\Omega}}_0\times\mathbf{s}/(\hat{\mathbf{\Omega}}_0\cdot\mathbf{s} - s_0), \tag{5}$$

where $s_0\hat{\mathbf{\Omega}}_0$ is an arbitrarily chosen vector in the order-parameter space $|\mathbf{s}| = s_0$. For this construction

$$f(\mathbf{A}(\mathbf{s})) = 4\pi\delta^2(\hat{\mathbf{\Omega}}_0, \mathbf{s}/s_0), \tag{6}$$

where $\delta^2(\hat{\mathbf{\Omega}}, \hat{\mathbf{\Omega}}')$ is the Dirac delta function on the unit sphere. The "vector potential" (5) thus has a Dirac string along the direction $\hat{\mathbf{\Omega}}_0$, which breaks rotational invariance. This expression for P has the equation of motion

$$\partial_t P = 4\pi s_0 \textstyle\sum_i \delta(t-t_i)\,\mathrm{sgn}[\mathbf{s}(x_i,t_i)\cdot\partial_t\mathbf{s}(x_i,t_i)\times\partial_x\mathbf{s}(x_i,t_i)], \tag{7}$$

where (x_i,t_i) are the space-time coordinates at which $\hat{\mathbf{\Omega}}_0\cdot\mathbf{s} = s_0$. The value of P defined with (5) jumps by the discrete amount $\pm 4\pi s_0$ each time the motion of the spin configuration $\mathbf{s}(x,t)$ sweeps across the singular point $\mathbf{s} = s_0\hat{\mathbf{\Omega}}_0$. The usual construction for P is thus only a valid momentum functional *if* the additional constraint that $\mathbf{s}(x,t)$ *never* takes the singular value $s_0\hat{\mathbf{\Omega}}_0$ is imposed. This is satisfied by solutions of the integrable model[1] corresponding to a single soliton moving on the ordered background $\mathbf{s}(x) = -s_0\hat{\mathbf{\Omega}}_0$, but is violated during the time evolution of general (multisoliton) configurations.

The expression (1) for P can be reexpressed as an integral around a closed path Γ in the *order-parameter* space:

$$P = \oint_\Gamma \mathbf{A}(\mathbf{s}) \cdot d\mathbf{s}. \tag{8}$$

Here Γ is the curve in the order-parameter space traced out by the instantaneous spin configuration, and is closed if the usual boundary conditions [either periodic, or $\mathbf{s}(-\infty) = \mathbf{s}(+\infty)$] are imposed. If the form (5) for $\mathbf{A}$ is used, P can be expressed by means of Stokes's theorem as the functional $s_0 \omega_P(\{\mathbf{s}(x)\})$, where ω_P is the solid angle[3] subtended by a surface in order-parameter space bounded by Γ, which does not include the singular point of (5).

This last condition uniquely fixes the surface integral in order-parameter space, but if it is relaxed, topologically different choices of the surface bounded by Γ lead to alternative values of ω_P differing by multiples of 4π. Consider now the functional

$$T_S = \exp(-iS\omega_P), \tag{9}$$

where $2S$ is *integral.* This is uniquely defined by the configuration Γ, independent of how the surface bounded by Γ is chosen. Furthermore, this is an explicitly rotationally invariant geometrical construction, and has no jumps in value as Γ sweeps though the singular point, and so it is a true constant of the motion. The functional T_S obeys the Poisson-bracket algebra

$$\{T_S, \mathbf{s}(x)\} = -i(S/s_0) T_S \partial_x \mathbf{s}(x). \tag{10}$$

While $T_{1/2}$ is a constant of the motion of the continuum classical model, there is a discrete set $T_S = (T_{1/2})^{2S}$ of other possible candidates for the fundamental translation-generating functional. It is natural to anticipate that T_S is the analog in the classical continuum model of the lattice translation operator $\hat{T}$ of the discrete spin-S quantum chain. In the classical model, s_0 is the magnitude of the spin density in the fully aligned state, and corresponds to $\hbar S/a$ in the spin-S quantum chain with lattice spacing a. The quantum lattice translation operator obeys the commutation relation $[\hat{T}, \hat{\mathbf{S}}_n] = (\hat{\mathbf{S}}_{n+1} - \hat{\mathbf{S}}_n)\hat{T}$; application of the correspondence principle and comparison with (10) leads to the identification of $\hat{T}$ with T_S.

A more precise derivation can be constructed by use of the continuum limit of the coherent-state description of the quantum chain discussed by Balakrishnan and Bishop (BB).[4] The translation operator of the quantum chain is not given by a simple expression, but can be explicitly written as

$$\hat{T} = \mathrm{Tr}[R(\hat{\mathbf{S}}_1) R(\hat{\mathbf{S}}_2) \cdots R(\hat{\mathbf{S}}_N)], \tag{11}$$

where periodic boundary conditions on a chain of N spins is assumed. $R(\hat{\mathbf{S}})$ is a $(2S+1)\times(2S+1)$ matrix operator with elements $R_{mm'}(\hat{\mathbf{S}}) = |m\rangle\langle m'|$, where $|m\rangle$ is an orthonormal basis of states of a single spin (e.g., eigenstates of S^z). Following BB, I describe the spin chain in terms of the overcomplete basis of coherent spin states $|\hat{\mathbf{\Omega}}_1, \mathbf{\Omega}_2, \ldots, \hat{\mathbf{\Omega}}_N\rangle$, where $|\hat{\mathbf{\Omega}}\rangle$ is the coherent state of a single spin, satisfying $\hat{\mathbf{\Omega}} \cdot \hat{\mathbf{S}} |\hat{\mathbf{\Omega}}\rangle = \hbar S |\hat{\mathbf{\Omega}}\rangle$. In the coherent-state basis, any operator is fully specified in terms of its diagonal matrix elements. For example, BB showed that taking the continuum limit of the diagonal coherent-state matrix element of the quantum-spin operator equation of motion yields the classical equation of motion of the continuum model. Applying this technique to powers of the translation operator gives

$$\langle \{\hat{\mathbf{\Omega}}_n\} | \hat{T}^m | \{\hat{\mathbf{\Omega}}_n\}\rangle = \prod_n \langle \hat{\mathbf{\Omega}}_n | \hat{\mathbf{\Omega}}_{n-m}\rangle. \tag{12}$$

The coherent state $|\hat{\mathbf{\Omega}}\rangle$ can be represented in terms of the orthonormal basis of eigenstates $|m\rangle$ of S^z through

$$\langle m | \hat{\mathbf{\Omega}}\rangle = \left[\frac{2S!}{(S+m)!(S-m)!}\right]^{1/2} \alpha^{S+m} \beta^{S-m}, \tag{13}$$

where $(\alpha^*, \beta^*) = \boldsymbol{\xi}^*$ are spinor coordinates satisfying $(\boldsymbol{\xi}^*, \boldsymbol{\xi}) = 1$, $(\boldsymbol{\xi}^*, \sigma^i \boldsymbol{\xi}) = \hat{\Omega}^i$, σ^i being the Pauli matrices. The overlap $\langle \hat{\mathbf{\Omega}}_1 | \hat{\mathbf{\Omega}}_2\rangle$ is given by $(\xi_1^*, \xi_2)^{2S}$. If ξ_n is represented by a continuous function $\xi(x_n)$, where $x_n = na$, and then a gradient expansion is made, we obtain

$$\langle \{\hat{\mathbf{\Omega}}(x)\} | \hat{T}^m | \{\hat{\mathbf{\Omega}}(x)\}\rangle = \exp[-2Sm \int dx (\xi^*(x), \partial_x \xi(x)) + O(a)]. \tag{14}$$

If the explicit representation $\boldsymbol{\xi}^* = (\cos(\tfrac{1}{2}\theta), \sin(\tfrac{1}{2}\theta) \times \exp(-i\phi))$ is substituted into (14), as $a \to 0$ the right-hand side of (14) becomes $\exp(-iSmP/s_0)$ where P is defined with use of the vector potential (5) with $\hat{\mathbf{\Omega}}_0 \cdot \mathbf{s} = -s_0 \cos\theta$; other representations of ξ related to this one by a gauge transformation $\boldsymbol{\xi} \to \exp(i\chi)\boldsymbol{\xi}$ change $P \to P + 2s_0 \int dx\, \partial_x \chi$. Periodic boundary conditions on $\xi(x)$ require periodic boundary conditions on $\exp(i\chi)$, and so the gauge transformation can only change the value of P by a multiple of $4\pi s_0$. Thus

$$\lim_{a\to 0} \langle \{\hat{\mathbf{\Omega}}(x_n)\} | \hat{T}^m | \{\hat{\mathbf{\Omega}}(x_n)\}\rangle = (T_S)^m, \tag{15}$$

independent of gauge transformations of $\boldsymbol{\xi}$.

Since a coherent state is not an eigenstate of the translation operator, it is a superposition of crystal-momentum eigenstates characterized by the distribution

$$\rho(ka)=\frac{1}{2\pi}\sum_{m=-\infty}^{+\infty} e^{imka}\langle \hat{T}^m\rangle. \quad (16)$$

The relation (15) implies that in the continuum limit when the coherent-state variables $\hat{\Omega}_n$ vary infinitely slowly on the scale of the lattice spacing, $\langle \hat{T}^m\rangle \to (\langle \hat{T}\rangle)^m$, and the crystal momentum distribution $\rho(ka)$ of the coherent state becomes a periodic delta function with its weight at $ka = S\omega_P$ plus multiples of 2π.

I note in passing that in their recent Letter,[4] BB did not consider the quantum translation operator $\hat{T}$, but introduced an *ad hoc Ansatz* for a "quantum analog of momentum":

$$\hat{P}=(\hbar/2a)\sum_n(\hat{S}_n^x\hat{S}_{n+1}^y-\hat{S}_{n+1}^x\hat{S}_n^y)/\gamma_n+\text{H.c.},$$

where $\gamma_n=[S(S+1)]^{1/2}+\hat{S}_n^z$. This quantity is not rotationally invariant (it does not commute with the total spin operators $S^{\pm}$) and the ordering of γ_n^{-1} is ambiguous; furthermore, it is quite unrelated to the rotationally invariant translation operator $\hat{T}$. The apparent motivation of this *Ansatz* is that in the continuum limit *and* the limit $S\to\infty$, its coherent-state expectation value reduces to the usual expression for P, using (5) with $\hat{\Omega}_0=-\hat{\mathbf{z}}$. Taking the continuum limit of its coherent-state expectation value, *but keeping S finite,* and evaluating this expression for a soliton solution of the classical model, BB claim to obtain finite-S "quantum corrections" to the soliton dispersion of the quantum chain. In fact, the correct treatment of the continuum limit of the translation operator given here indicates that the only S dependence in the continuum limit is that the crystal momentum ka is $S\omega_P$. A variant of the spin-S Heisenberg chain is exactly solvable by the Bethe *Ansatz,*[5] and the dispersion relations of the single-soliton excitations[6] do *not* exhibit the "novel features" claimed by BB, which appear to be purely the result of an invalid construction of a "quantum analog of momentum" for the spin chain.

For $S>\frac{1}{2}$, the dispersion relation of the semiclassically quantized single-soliton excitations parametrized by ω_P or $T_{1/2}$ spans $2S$ consecutive Brillouin zones, without a gap at the intervening zone boundaries. This feature is also found in the exactly solvable quantum model,[6] but in general umklapp processes which are lost in the continuum limit will open gaps at the zone boundaries, and only T_S, not $T_{1/2}$, will correspond to a conserved quantity of the quantum chain. In addition, a restriction that soliton solutions of the continuum model that vary on length scales smaller than the effective lattice spacing $a=\hbar S/s_0$ are not physical must be imposed. As I have noted some time ago,[7] a soliton carrying spin deviation $m\hbar$ can be regarded as a bound state of m elementary solitons, each carrying spin deviation $\hbar$, and can be associated with a "wave number" parameter $Q=s_0\omega_P/m\hbar$. The physical restriction is then equivalent to the selection rule $|Q|\leq\pi/a$ on physical soliton states. This means that while the general soliton dispersion covers $2S$ consecutive Brillouin zones, the solitons with $m<2S$ have a dispersion covering only m consecutive zones, consistent with the identification of the $m=1$ soliton with the elementary magnon of the spin chain. This prediction[7] was subsequently verified[6] in the spectrum of the solvable spin-S model.[5]

The classical continuum description of single-soliton states will be valid in the long-wavelength limit, $|Qa|=|S\omega_P/m|<<1$, where $|\omega_P|\leq 2\pi$. Trivially, this is satisfied in the small-spin-deviation limit, $|\omega_P|<<2\pi$. More generally, it is always satisfied in the "semiclassical limit" $m>>2S$; the semiclassically quantized model[7] and the Bethe-*Ansatz*–solvable model[6] have identical spectra in this limit, but quantitative deviations are important for $m\lesssim 2S$.

In conclusion, I have resolved a long-standing paradox involving the nonexistence of a rotationally invariant momentum functional for the classical continuum model of a one-dimensional Heisenberg ferromagnet by showing that there is *no* such quantity in *either* the classical model *or* the equivalent discrete-spin quantum chain. Instead, the conserved quantity associated with translational invariance of the classical model is an analog of the quantum lattice translation operator, and has a rotationally invariant geometrical interpretation in terms of the solid angle subtended by the spin-density field in the order-parameter space. This quantity exhibits a topological quantization parametrized by an integer or half-integer number S which corresponds to the spin quantum number of the associated quantum spin chain. "Novel S-dependent quantum corrections" to the soliton excitations of the quantum chain reported in a recent Letter[4] are found to be artifacts of the use of an invalid *Ansatz* for an analog of "momentum" in the quantum chain. The classical continuum model is identified precisely as the model defined by the equations obtained by taking a continuum limit of diagonal matrix elements of operator equations of the discrete quantum model in the overcomplete spin-coherent state basis, rather than involving a classical limit $S\to\infty$. It is an accurate description of "semiclassical" soliton states where the spin-deviation quantum number m is much larger than $2S$. "Quantum corrections" to the semiclassically quantized solutions of the continuum model must be sought in terms (such as umklapp processes) that do not survive the continuum limit.

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