Spin-Wave Dynamics in Real Crystals

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We derive the spin-wave dynamics in crystals from the time-dependent variational principle, which involves Berry phase terms as well as the energy of frozen spin waves. The general formulation is based on the adiabatic and harmonic approximations. Formulas for ferromagnets and antiferromagnets are derived in terms of Kohn-Sham wave functions, which are particularly suitable for practical *ab initio* calculations. [S0031-9007(98)05490-8]

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In spite of the fact that when applied to itinerant electrons, the Heisenberg Hamiltonian is at best only a parametrized model, all calculations of spin-wave dispersion curves have to this day been based on that venerable model [1]. This is exemplified in a recent monograph where Aharoni [2] chooses "to use the assumption of localized magnetic moments on lattice sites, and the Heisenberg Hamiltonian, because it is the only way to include the variation of the magnetization in space." Contrary to this widely held belief, in this Letter we derive spin-wave equations of motion which in the harmonic and adiabatic limit are exact everywhere between the localized moment and jellium limits, and are universally applicable to ferromagnets, antiferromagnets, and ferrimagnets. We then show how the quantities appearing in the equations of motion can be exactly evaluated within density functional theory [3], which is known to yield accurate values for the ground state magnetization of Fe, Co, and Ni. Interestingly, the formulas for the ferromagnetic spin-wave frequency, when written in terms of the frozen spin-wave energy, become identical in the jellium and localized limits.

General formulation.—Suppose we have a symmetry broken ground state $|\psi_0\rangle$ with a magnetization density $m(\mathbf{r})\hat{\mathbf{e}}(\mathbf{r}) = \langle\psi_0|\hat{\rho}(\mathbf{r})\boldsymbol{\sigma}|\psi_0\rangle$, where $\boldsymbol{\sigma}$ is the Pauli matrix vector and $\hat{\rho}(\mathbf{r})$ is the density operator. The direction $\hat{\mathbf{e}}(\mathbf{r})$ (constant for a ferromagnet) may be a function of position in general, but we assume it has a periodicity commensurate with the crystal lattice, while $|\psi_0\rangle$ has the periodicity of the magnetic lattice defined by $m(\mathbf{r})\hat{\mathbf{e}}(\mathbf{r})$. With the excitation of a spin wave, the magnetization density becomes $m(\mathbf{r})[\hat{\mathbf{e}}(\mathbf{r}) + \mathbf{S}(\mathbf{r})]$, where for a small amplitude of $\mathbf{S}(\mathbf{r})$ we can write the spin wave in the form

$$\mathbf{S}(\mathbf{r}) = \mathrm{Re}\left\{e^{i\mathbf{k}\cdot\mathbf{r}}\sum_{\mathbf{G}}\mathbf{S}_{\mathbf{G}}e^{i\mathbf{G}\cdot\mathbf{r}}\right\}, \tag{1}$$

where the sum is over the reciprocal lattice vectors of the magnetic unit cell. Our task is to establish the equations of motion governing the time evolution of the spin-wave excitations. When these equations are linearized for small amplitudes, we should be able to obtain the normal modes and their frequency dispersions.

Our derivation of the spin dynamics is based on the adiabaticity assumption that the electronic wave function can always follow the instantaneous spin-wave configuration [4]. We first introduce a frozen spin-wave state $|\psi\rangle$ defined as the lowest energy state with a given spin-wave configuration $m(\mathbf{r})[\hat{\mathbf{e}}(\mathbf{r}) + \mathbf{S}(\mathbf{r})] = \langle\psi|\hat{\rho}(\mathbf{r})\boldsymbol{\sigma}|\psi\rangle$. This makes $|\psi\rangle$ a functional of $\mathbf{S}(\mathbf{r})$ or a function of its Fourier components $\mathbf{S}_{\mathbf{G}}$. Then we demand that $\mathbf{S}_{\mathbf{G}}$ should evolve with time in such a way that the adiabatic wave function $e^{if(t)}|\psi[\mathbf{S}_{\mathbf{G}}(t)]\rangle$ satisfies the time-dependent Schrödinger equation for some phase $f(t)$.

This requirement can be conveniently implemented by employing the time-dependent variational principle that the action $\int L\,dt$ should be extremized by physical wave functions, where $L = \langle\Psi|i\hbar\frac{\partial}{\partial t}|\Psi\rangle - \langle\Psi|H|\Psi\rangle$. When we substitute the adiabatic wave function into this expression, we obtain a Lagrangian for the variables $\mathbf{S}_{\mathbf{G}}$,

$$L = \hbar\sum_{\mathbf{G}j}\dot{S}^j_{\mathbf{G}}\langle\psi|\frac{i\partial}{\partial S^j_{\mathbf{G}}}|\psi\rangle - E\,, \tag{2}$$

where the dot on $S^j_{\mathbf{G}}$ indicates a time derivative, and $E = \langle\psi|H|\psi\rangle$ is the energy of the system for the given spin configuration. The variable $S^j_{\mathbf{G}}$ is the real or imaginary part of a vector component of $\mathbf{S}_{\mathbf{G}}$, and j is an index labeling the six different possibilities. The phase $f(t)$ in the adiabatic wave function only contributes a term of total time derivative, which we have dropped from the Lagrangian without any physical consequences [5]. The terms in the sum are related to the Berry phase of the adiabatic wave function, and their appearance is universal in adiabatic Lagrangians of slow variables [6].

The Euler-Lagrange equations for extremizing the action then governs the dynamics of these variables,

$$-\sum_{j',\mathbf{G}'}\hbar\Omega^{jj'}_{\mathbf{G}\mathbf{G}'}\dot{S}^{j'}_{\mathbf{G}'} + \frac{\partial E}{\partial S^j_{\mathbf{G}}} = 0\,, \tag{3}$$

where the Ω matrix (the Berry curvature) is defined as

$$\Omega^{jj'}_{\mathbf{G}\mathbf{G}'} = \frac{\partial}{\partial S^j_{\mathbf{G}}}\langle\psi|\frac{i\partial}{\partial S^{j'}_{\mathbf{G}'}}|\psi\rangle - \frac{\partial}{\partial S^{j'}_{\mathbf{G}'}}\langle\psi|\frac{i\partial}{\partial S^j_{\mathbf{G}}}|\psi\rangle\,. \tag{4}$$

Consistent with our assumption of small amplitudes, we make the harmonic approximation by linearizing the force $\partial E/\partial S^j_{\mathbf{G}}$, yielding

$$\sum_{j',\mathbf{G}'}[-\hbar\Omega^{jj'}_{\mathbf{G}\mathbf{G}'}\dot{S}^{j'}_{\mathbf{G}'} + K^{jj'}_{\mathbf{G}\mathbf{G}'}S^{j'}_{\mathbf{G}'}] = 0\,, \tag{5}$$

where $K^{jj'}_{\mathbf{G}\mathbf{G}'}$ is the second derivative of the energy E with respect to $S^j_{\mathbf{G}}$ and $S^{j'}_{\mathbf{G}'}$. Both Ω and K are evaluated at the ground state configuration, where the first derivatives of the energy vanish.

The above set of equations is a central result of this work, which in principle allows one to study the spin dynamics for a general many-body system. Since the spin variables are real, K is obviously real, and so is the Ω matrix [7]. Also, by definition, K is symmetric in the simultaneous interchange of $\mathbf{G}$ and j with $\mathbf{G}'$ and j', while Ω is antisymmetric. The secular equations for the normal modes are obtained by replacing the time derivative by $-i\omega$. The above properties of the matrices guarantee that the eigenfrequencies are real.

The elements of the K matrix may be obtained in a straightforward manner. Let $E(S^j_{\mathbf{G}})$ be the energy (relative to the ground state energy) in the state of the frozen spin configuration (1) with a single amplitude $S^j_{\mathbf{G}}$ present. Then we have $\frac{1}{2}K^{jj}_{\mathbf{G}\mathbf{G}}(S^j_{\mathbf{G}})^2 = E(S^j_{\mathbf{G}})$, from which the diagonal elements of the K matrix are obtained. To obtain the off-diagonal elements, let $E(S^j_{\mathbf{G}}, S^{j'}_{\mathbf{G}'})$ be the energy in the state of the frozen spin configuration (1) with the two spin amplitudes present. Then, $K^{jj'}_{\mathbf{G}\mathbf{G}'}S^j_{\mathbf{G}}S^{j'}_{\mathbf{G}'}$ is just the energy difference $E(S^j_{\mathbf{G}}, S^{j'}_{\mathbf{G}'}) - E(S^j_{\mathbf{G}}) - E(S^{j'}_{\mathbf{G}'})$.

The evaluation of the Ω matrix needs some consideration, but the final formula is straightforward to implement. For small amplitudes, the product $\frac{1}{2}\Omega^{jj'}_{\mathbf{G}\mathbf{G}'}S^j_{\mathbf{G}}S^{j'}_{\mathbf{G}'}$ is equal to the phase, or the imaginary part of the logarithm of the following quantity:

$$\langle\psi(0)|\psi(S^j_{\mathbf{G}})\rangle\langle\psi(S^j_{\mathbf{G}})|\psi(S^{j'}_{\mathbf{G}'})\rangle\langle\psi(S^{j'}_{\mathbf{G}'})|\psi(0)\rangle\,, \tag{6}$$

where $|\psi(0)\rangle$ is the ground state, and $|\psi(S^j_{\mathbf{G}})\rangle$ is the state with a single spin-wave amplitude $S^j_{\mathbf{G}}$. This result can be shown by a brute force expansion to quadratic order in the spin-wave amplitudes, bearing in mind that $\langle\psi|(\partial/\partial S)|\psi\rangle$ is purely imaginary [7]. The above result was motivated from a relation between the Berry curvature and the Berry phase [8].

The quantity (6) is quite suitable for numerical calculations, because one needs to deal only with wave functions of a single spin-wave amplitude. Also, because each wave function and its complex conjugate appears in the expression, one need not worry about the arbitrary phases of the wave functions [9]. Finally, if we choose the phases of the wave functions such that their projections on the ground state are real and positive, then the first and last factors in (6) may be dropped, yielding

$$\Omega^{jj'}_{\mathbf{G}\mathbf{G}'} = \frac{\text{phase of } \langle\psi(S^j_{\mathbf{G}})|\psi(S^{j'}_{\mathbf{G}'})\rangle}{\frac{1}{2}S^j_{\mathbf{G}}S^{j'}_{\mathbf{G}'}}\,. \tag{7}$$

Reduction by symmetries.—It has been a common practice to separate the dynamics of the transverse spin components from the longitudinal. This does not seem to be possible in the presence of spin-orbit coupling, unless the ground state magnetization and the Bloch wave vector of the spin wave lie along a crystal axis. In this Letter, we will consider the simpler situation where spin-orbit coupling is neglected. Then the ground state magnetization is along a fixed direction, say, the z direction ($+z$ and $-z$ for an antiferromagnet), and the matrices Ω and K are invariant under spin rotations about the z axis, with the following consequences: (i) All the matrix elements coupling the z with the x and y components must vanish; (ii) the xx and the yy elements of the matrices are equal; and (iii) the xy and yx elements of the matrices differ only by a sign. Because of these properties, the spin dynamics of $S^x + iS^y$, $S^x - iS^y$, and S^z are mutually decoupled. Moreover, the spectra of the two transverse polarizations are simply related by time reversal.

In the rest of this Letter, we will be concerned with one of the transverse modes, which is known to have a spectral branch (Goldstone mode) whose frequency vanishes as $\mathbf{k} \to 0$. Our spin wave (1) will be restricted to the form

$$\mathbf{S}(\mathbf{r}) = \mathrm{Re}\left\{e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}\sum_{\mathbf{G}}(\hat{\mathbf{x}} + i\hat{\mathbf{y}})S_{\mathbf{G}}e^{i\mathbf{G}\cdot\mathbf{r}}\right\}. \tag{8}$$

Using the new independent variables $S^1_{\mathbf{G}} = \mathrm{Re}\,S_{\mathbf{G}}$ and $S^2_{\mathbf{G}} = \mathrm{Im}\,S_{\mathbf{G}}$, we can now repeat the calculations through Eq. (7) without changing any formulas, except that the superscript j now labels the two possibilities instead of the previous six.

Further simplifications are achieved by the observation that a spin rotation about the z axis is equivalent to a phase change of the amplitude $S_{\mathbf{G}}$, that is, a rotation between the real and imaginary parts. Therefore, invariance of the Ω and K matrices under the spin rotation implies that $\Omega^{11}_{\mathbf{G}\mathbf{G}'} = \Omega^{22}_{\mathbf{G}\mathbf{G}'}$ and $\Omega^{12}_{\mathbf{G}\mathbf{G}'} = -\Omega^{21}_{\mathbf{G}\mathbf{G}'}$, with the same relations for K. Because of these, the variables $S_{\mathbf{G}} = S^1_{\mathbf{G}} + iS^2_{\mathbf{G}}$ and its complex conjugate are decoupled, and the equations of motion (5) are reduced to

$$\sum_{\mathbf{G}'}[i\hbar\omega\Omega_{\mathbf{G}\mathbf{G}'} + K_{\mathbf{G}\mathbf{G}'}]S_{\mathbf{G}'} = 0\,, \tag{9}$$

where we have replaced the time derivative by $-i\omega$. The new matrices are defined as $\Omega_{\mathbf{G}\mathbf{G}'} = \Omega^{11}_{\mathbf{G}\mathbf{G}'} - i\Omega^{12}_{\mathbf{G}\mathbf{G}'}$ and $K_{\mathbf{G}\mathbf{G}'} = K^{11}_{\mathbf{G}\mathbf{G}'} - iK^{12}_{\mathbf{G}\mathbf{G}'}$. Because of the symmetry properties among the matrix elements mentioned above and earlier [the paragraph below that of Eq. (5)], the new K matrix is Hermitian, $K^*_{\mathbf{G}'\mathbf{G}} = K_{\mathbf{G}\mathbf{G}'}$, while the new Ω matrix is anti-Hermitian, $\Omega^*_{\mathbf{G}'\mathbf{G}} = -\Omega_{\mathbf{G}\mathbf{G}'}$. This implies that for $\mathbf{G}' = \mathbf{G}$, $K^{12}_{\mathbf{G}\mathbf{G}}$ and $\Omega^{11}_{\mathbf{G}\mathbf{G}}$ vanish.

Kohn-Sham.—We now consider how our formalism may be implemented in the Kohn-Sham density functional theory [3], in which the many-body wave function is represented by a determinant of single particle states. In the absence of spin-orbit coupling, the single particle states in the ground state of the system may be taken as either spin up, or spin down, with the spatial wave functions being Bloch waves. To fix ideas, we consider how a spin-up state mixes with a spin-down component, when the magnetization is tilted away from the z axis due to a spin wave of wave vector $\mathbf{k}$ and amplitude $S^j_{\mathbf{G}}$ [10]. The spin-density functional theory dictates that the Kohn-Sham potential becomes a position dependent matrix whose eigenspinors line up with the local magnetization direction [11,12]. Thanks to an insight by Herring [13], one can show that the potential matrix and thus the Kohn-Sham Hamiltonian are invariant under a lattice translation combined with a spin rotation. This leaves the wave function in the form $|u(S^j_{\mathbf{G}})\rangle|\uparrow\rangle + |v(S^j_{\mathbf{G}})\rangle|\downarrow\rangle$, where $|u\rangle$ and $e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}}|v\rangle$ are Bloch waves [14] which can be calculated using standard band structure techniques.

The K matrix can be obtained from standard procedures for the energetics of the frozen spin-wave states, so we will focus on the calculation of the Ω matrix. It is straightforward to show that the Berry curvature of the many-body wave function is equal to the sum of Berry curvatures of the occupied states [15]. The same kind of reasoning leading to Eqs. (6) and (7) can be applied to a single particle state. Therefore, the contribution to $\Omega^{jj'}_{\mathbf{G}\mathbf{G}'}$ from a spin-up state is the phase of

$$\langle u(S^j_{\mathbf{G}})|u(S^{j'}_{\mathbf{G}'})\rangle + \langle v(S^j_{\mathbf{G}})|v(S^{j'}_{\mathbf{G}'})\rangle \tag{10}$$

divided by $\frac{1}{2}S^j_{\mathbf{G}}S^{j'}_{\mathbf{G}'}$. It is understood that this formula should be used after choosing the phases of $|u(S)\rangle$, $\{S = S^j_{\mathbf{G}}, S^{j'}_{\mathbf{G}'}\}$, such that the projections $\langle u(0)|u(S)\rangle$ are real and positive. Consistent with this condition and to second order in the spin-wave amplitudes, the phase of (10) is equal to the imaginary part of $\langle v(S^j_{\mathbf{G}})|v(S^{j'}_{\mathbf{G}'})\rangle$ [16]. This shows that when the amplitudes $S^2_{\mathbf{G}'}$ and $S^1_{\mathbf{G}'}$ are given the same value, the contribution to $\Omega_{\mathbf{G}\mathbf{G}'} \equiv \Omega^{11}_{\mathbf{G}\mathbf{G}'} - i\Omega^{12}_{\mathbf{G}\mathbf{G}'}$ from the spin-up state may be written as

$$\mathrm{Im}\langle v(S^1_{\mathbf{G}})|v(S^1_{\mathbf{G}'})\rangle - i\,\mathrm{Im}\langle v(S^1_{\mathbf{G}})|v(S^2_{\mathbf{G}'})\rangle \tag{11}$$

divided by $\frac{1}{2}S^1_{\mathbf{G}}S^1_{\mathbf{G}'}$. This is just $i\langle v(S^1_{\mathbf{G}})|v(S^1_{\mathbf{G}'})\rangle^* = i\langle v(S^1_{\mathbf{G}'})|v(S^1_{\mathbf{G}})\rangle$, because of the relation $|v(S^2_{\mathbf{G}'})\rangle = e^{-i(\pi/2)}|v(S^1_{\mathbf{G}'})\rangle$ [17]. Finally, after a similar consideration for spin-down states, we find that $\Omega_{\mathbf{G}\mathbf{G}'}$ is given by

$$\Omega_{\mathbf{G}\mathbf{G}'} = \frac{i\sum[\langle v(S^1_{\mathbf{G}'})|v(S^1_{\mathbf{G}})\rangle_\uparrow - \langle u(S^1_{\mathbf{G}'})|u(S^1_{\mathbf{G}})\rangle_\downarrow]}{\frac{1}{2}S^1_{\mathbf{G}}S^1_{\mathbf{G}'}}, \tag{12}$$

where the sum is over the occupied single particle states, and the arrows indicate the spin orientation of the state in the absence of the spin wave [18].

The almost-jellium regime.—Here, the lowest branch of the spin waves is dominated by the $\mathbf{G} = 0$ Fourier component except near the zone boundary. Then, we can immediately solve for the eigenfrequency from (9) as

$$\hbar\omega = \frac{K_{00}}{-i\Omega_{00}} = \frac{\frac{1}{2}K^{11}_{00}(S^1_0)^2}{\sum[\langle v|v\rangle_\uparrow - \langle u|u\rangle_\downarrow]}, \tag{13}$$

using (12) with $\mathbf{G} = \mathbf{G}' = 0$. As previously discussed, the numerator is just the energy $\Delta E(\mathbf{k})$ to create the spin wave. The denominator is simply the reduction of the total crystal spin S due to the spin wave, because $\sum\langle v|v\rangle_\uparrow$ represents the reduction of the up component of the spin-up electrons and $\langle u|u\rangle_\downarrow$ represents the reduction of the down component of the spin-down electrons. Therefore, we have the more transparent result

$$\hbar\omega = 2\Delta E(\mathbf{k})/S\theta^2, \tag{14}$$

where θ is the angle of tilt of the local magnetization from the z direction.

Several remarks are in order. First, $\Delta E(\mathbf{k})$ is proportional to θ^2, so that ω is independent of tilt angle. Second, although $\Delta E(\mathbf{k})$ and S are total crystal quantities, we may also take them to be the spin-wave energy and net spin per unit cell. Third, at long wavelengths, the energy $\Delta E(\mathbf{k})$ is proportional to the square of the spin-density gradient, so that $\omega \propto k^2$. Finally, for a Heisenberg Hamiltonian with spin S per unit cell, one also obtains (14) [19], although the energy $\Delta E(\mathbf{k})$ for the two cases is not the same.

Near the Brillouin zone boundary, coupling between different Fourier components becomes important. At $\mathbf{k} = -\mathbf{G}/2$, the spin waves of amplitude S_0 and $S_{\mathbf{G}}$ have equal but opposite wave vectors, and they are degenerate because the 00 and $\mathbf{G}\mathbf{G}$ components are equal to each other for both the K and Ω matrices [20]. This degeneracy will be lifted to produce a gap at the zone edge when their coupling is taking into account

$$\begin{aligned}[i\hbar\omega\Omega_{00} + K_{00}]S_0 + [i\hbar\omega\Omega_{0\mathbf{G}} + K_{0\mathbf{G}}]S_{\mathbf{G}} = 0,\\ [i\hbar\omega\Omega_{\mathbf{G}0} + K_{\mathbf{G}0}]S_0 + [i\hbar\omega\Omega_{\mathbf{G}\mathbf{G}} + K_{\mathbf{G}\mathbf{G}}]S_{\mathbf{G}} = 0.\end{aligned} \tag{15}$$

In addition, if the ground state has space inversion symmetry, then the $0\mathbf{G}$ and $\mathbf{G}0$ components are also equal for both the K and Ω matrices [21]. Because of the Hermiticity of K and anti-Hermiticity of Ω, the above symmetry arguments imply that the elements K^{12}_{00}, $K^{12}_{0\mathbf{G}}$, Ω^{11}_{00}, and $\Omega^{11}_{0\mathbf{G}}$ all vanish. Thus,

$$\hbar\omega = \frac{K_{00} \pm K_{0\mathbf{G}}}{i(\Omega_{00} \pm \Omega_{0\mathbf{G}})} = \frac{K^{11}_{00} \pm K^{11}_{0\mathbf{G}}}{\Omega^{12}_{00} \pm \Omega^{12}_{0\mathbf{G}}}. \tag{16}$$

In the case of an antiferromagnetic ground state, the denominators in (13) and (14) vanish, so it is essential to include other Fourier components of the spin wave even for $\mathbf{k}$ away from the zone boundary. For this purpose, we consider the effect of coupling to a single $\mathbf{G}$ of

minimal size for which the spin-wave changes sign under translations connecting the up and down spin sublattices. In this case, the matrix elements Ω_{00}, $\Omega_{\mathbf{GG}}$, and $K_{0\mathbf{G}}$ are zero [22], with which Eq. (15) yields

$$\hbar\omega = \frac{\sqrt{K_{00}K_{\mathbf{GG}}}}{|\Omega_{0\mathbf{G}}|}, \tag{17}$$

where we have used the relation $\Omega_{\mathbf{G}0} = -\Omega_{0\mathbf{G}}^{*}$.

The above result confirms the usual behavior for antiferromagnetic spin waves that $\omega \propto k$ as $\mathbf{k} \to 0$, because K_{00} is of order k^2, while $K_{\mathbf{GG}}$ and $\Omega_{0\mathbf{G}}$ approach finite constants. This qualitative result remains true even if the coupling to other Fourier components is included, although the frequency may be changed quantitatively.

In summary, within the adiabatic and harmonic approximations, we have obtained the exact spin-wave equations of motion for any ferromagnetic, ferrimagnetic, or antiferromagnetic crystal. We showed how to evaluate the parameters therein in both the many-body and the one electron pictures. We also demonstrated that the frequency has the correct $\mathbf{k}$ dependence at small k and at the zone boundary for both the ferromagnetic and antiferromagnetic crystals.

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[7] The quantity $\langle\psi|(\partial/\partial S)|\psi\rangle$ is purely imaginary, because the sum of its complex conjugate and itself is just the derivative of $\langle\psi|\psi\rangle = 1$.

[8] The quantity $\frac{1}{2}\Omega_{\mathbf{GG}'}^{jj'}S_{\mathbf{G}}^{j}S_{\mathbf{G}'}^{j'}$ may be regarded as an areal integral of $\Omega_{\mathbf{GG}'}^{jj'}$ inside the right triangle in the $S_{\mathbf{G}}^{j} - S_{\mathbf{G}'}^{j'}$ plane whose corners are at (0,0), $(S_{\mathbf{G}}^{j}, 0)$, and $(0, S_{\mathbf{G}'}^{j'})$. In view of Eq. (4) and Stokes's theorem, this may be turned into a line integral of the vector $\langle\psi|(i\partial/\partial\mathbf{S})|\psi\rangle$ along the sides of the triangle. This is just the Berry phase around the triangle, which coincides with the phase of the expression (6) when the triangle is small.

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[14] In order to keep the wave function continuous at zero spin-wave amplitude which is necessary for the Berry curvature calculations later, the spin rotation operator about the z axis used in [11,12] is modified into the form $e^{i\phi(\sigma_z-1)/2}$, where σ_z is the z component Pauli matrix, and $\phi = (\mathbf{k} + \mathbf{G}) \cdot \mathbf{r}$ is the angle of rotation.

[15] The easiest way to prove this is to show the same statement for the quantity $\langle\psi|(\partial/\partial S_{\mathbf{G}}^{j})|\psi\rangle$. Since the derivative acts separately on the single particle wave functions, it may be regarded as a sum of single particle operators.

[16] In the presence of a spin wave, the potential matrix has off-diagonal elements first order in the spin-wave amplitude, while the diagonal elements differ from the unperturbed one only in second order. Moreover, we have required $\langle u(0)|u(S)\rangle$ to be real and positive. Therefore, $|v(S)\rangle$ is of first order in the spin-wave amplitude S, and $|u(S)\rangle - |u(0)\rangle$ is of second order.

[17] The spin wave of amplitude $S_{\mathbf{G}} = iS_{\mathbf{G}}^{2}$ can be obtained from a spin wave of amplitude $S_{\mathbf{G}} = S_{\mathbf{G}}^{1}$ by a spin rotation. Applying the spin rotation operator in Ref. [14] with $\phi = -\pi/2$, we obtain the relation in the text.

[18] In the atomic sphere approximation [11,12] where the direction of magnetization is taken to be constant over each Wigner-Seitz sphere, $\mathbf{k}$ and $\mathbf{k} + \mathbf{G}$ are equivalent, so $\mathbf{G}$'s other than $\mathbf{G} = 0$ are redundant. In a full potential calculation, one can force a spin wave with $S_{\mathbf{G}}$ as its main component, but self-consistency will cause it to be dressed with other Fourier components of smaller amplitude. Equation (12) still holds for the dressed spin-wave amplitudes with the understanding that $S_{\mathbf{G}}$ stands for the amplitude of the main component of a spin wave.

[19] Although it can be shown in general, here we show it for a nearest neighbor linear chain. Following C. Kittel [*Introduction to Solid State Physics* (Wiley, New York, 1996), 7th ed.], we have $\hbar\omega = 4JS(1 - \cos ka)$, whereas $E(k) = -2J\mathbf{S}_p \cdot \mathbf{S}_{p+1} = -2J(S_z^2 + S_\perp^2 \cos ka)$ and $\Delta E = E(k) - E(0) = 2JS_\perp^2(1 - \cos ka) \approx 2JS^2\theta^2(1 - \cos ka)$.

[20] The ground state is invariant under complex conjugation which is equivalent to time reversal followed by a spin rotation of 180° about the y axis. For a spin-wave state with $\mathbf{k} = -\mathbf{G}/2$, this operation reflects the spin y component, and thus replaces the roles of S_0 and $S_{\mathbf{G}}$ by $S_{\mathbf{G}}^{*}$ and S_0^{*}, respectively.

[21] Under space inversion, the roles played by S_0 and $S_{\mathbf{G}}$ are interchanged. Therefore, the matrix elements of K and Ω must be invariant under $0 \leftrightarrow \mathbf{G}$.

[22] In the presence of spin waves of amplitude S_0 and $S_{\mathbf{G}}$, the energy above the ground state equals half of $K_{00}|S_0|^2 + K_{0\mathbf{G}}S_0^{*}S_{\mathbf{G}} + K_{\mathbf{G}0}S_{\mathbf{G}}^{*}S_0 + K_{\mathbf{GG}}|S_{\mathbf{G}}|^2$. Under the symmetry operation of time reversal followed by the translation $\mathbf{r} \to \mathbf{r} + \mathbf{R}/2$ between the sublattices, the spin-wave amplitude S_0 changes a phase of $\mathbf{k} \cdot \mathbf{R}/2$, while $S_{\mathbf{G}}$ changes a phase of $(\mathbf{k} + \mathbf{G}) \cdot \mathbf{R}/2$. The extra phase in $S_{\mathbf{G}}$ makes the second and third terms of the energy switch their signs. In order for the energy to be invariant under the symmetry operation, these terms must vanish for arbitrary S_0 and $S_{\mathbf{G}}$, which implies the vanishing of $K_{0\mathbf{G}}$.