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Phase Locking in the Heisenberg Helimagnet

Abstract

The commensurability energy ΔE is calculated for a Heisenberg helimagnet whose wavelength is three lattice constants at zero temperature with a small but nonzero uniform field applied in the plane of polarization of the spins. It is shown that $\Delta E=0$ for classical spins but $\Delta E \neq 0$ for quantum spins when spin-wave interactions are considered.

Disciplines

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Phase locking in the Heisenberg helimagnet

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The commensurability energy ΔE is calculated for a Heisenberg helimagnet whose wavelength is three lattice constants at zero temperature with a small but nonzero uniform field applied in the plane of polarization of the spins. It is shown that $\Delta E=0$ for classical spins but $\Delta E \neq 0$ for quantum spins when spin-wave interactions are considered.

In this paper it is shown that phase locking occurs in a broad class of Heisenberg helimagnets when a uniform field is applied in the plane of polarization. The model Hamiltonian I treat is¹

$$\mathcal{H} = \frac{1}{2} \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j - h \sum_i S_{ix} + \epsilon \sum_i S_{iz}^2 \quad (1a)$$

$$= \mathcal{H}_{Ex} + \mathcal{H}_Z + \mathcal{H}_A, \quad (1b)$$

where $\mathbf{S}_i$ is a quantum spin of magnitude S on the i th site of a simple tetragonal lattice. I include a small easy plane anisotropy energy ϵ whose effect is to orient the spins in the x - y plane but can otherwise be neglected in the limit of small h . Arbitrarily I take the x - y plane to coincide with the a - b plane. Also $J_{ij} = J(\mathbf{r}_i - \mathbf{r}_j)$ is assumed to have the symmetry of the lattice. In the a - b plane interactions between first, second, and third nearest neighbors are, respectively, $j_1 = 1$, j_2 , and j_3 . For nearest neighbors in the c direction, $J_{ij} = J_1 > 0$. All other interactions are neglected. For sufficiently negative values of j_2 and/or j_3 the classical ground state of this model is¹ a helix of wave vector $\mathbf{Q} \neq 0$. For $h=0$ the value of $\mathbf{Q}$ is a continuous function of j_2 and j_3 in contrast to the devil's staircase (i.e., stepwise discontinuous) behavior for the axial nearest, next-nearest-neighbor Ising (ANNNI) model.² Since the Heisenberg helix (for $h=0$) has a circular cross section, the free energy is clearly independent of the phase of the helix and the commensurability energy vanishes. On the other hand, application of a field in the plane of polarization distorts the cross section of the helix into an ellipse and leads to my results for $h \neq 0$ that the Heisenberg system exhibits an incomplete devil's staircase.

Early spin-wave calculations³⁻⁵ indicated the presence of a Goldstone mode for small h . This phason mode occurs if the energy is independent of the phase of the helix. This early work was based on linearized spin-wave theory and implied that $\mathbf{Q}$ varied continuously with j_2 and j_3 . Recently, it was shown⁶ that nonlinear spin-wave interactions modified this picture. For small h the pinning free energy (omitted in the early work) is of the form

$$\delta F = \sum_{p \geq 1; \mathbf{G}} A_p(T) h^p \delta(p\mathbf{Q} - \mathbf{G}) \cos p\phi, \quad (2)$$

where p is an integer, $\mathbf{G}$ a (big) reciprocal lattice vector, and ϕ the phase of the helix. Minimization with respect to ϕ yields

$$\delta F = - |A_p(T) h^p| \delta(p\mathbf{Q} - \mathbf{G}), \quad (3)$$

and consequently $\mathbf{Q}$ will remain pinned at the (commensurate) value $\mathbf{G}/p$ for a range of values of j_2 and j_3 of order $\Delta j_2 \sim \Delta j_3 \sim h^{p/2}$. This behavior is referred to as devil's staircase behavior and has been extensively studied in the Frenkel-Kontorova model.⁷ Previously⁶ we found $A_p(T)$ to be nonzero for a classical model except for the special case $p=3$, $T=0$. Some time ago Elliott and Lange⁴ showed explicitly that $A_3(T=0)=0$ for classical models within linear spin-wave theory. Our previous result for a classical model [$A_3(T=0) \sim T$] extended this result to include the effect of nonlinearity. In the present paper, however, it is shown that $A_3(T=0) \neq 0$ when quantum spin-wave interactions are included. Thus even for $p=3$, $A_p(T) = 0$ should be viewed as defining a special isolated multicritical point.

We now consider the calculation of $A_3(T=0)$ for a quantum spin system. Since this calculation is extremely complicated, it can only be summarized here. Following Ref. 8 one writes

$$S_i^x = -\sin(\mathbf{Q} \cdot \mathbf{r}_i + \phi) S_i^\eta + \cos(\mathbf{Q} \cdot \mathbf{r}_i + \phi) S_i^\xi, \quad (4a)$$

$$S_i^y = \cos(\mathbf{Q} \cdot \mathbf{r}_i + \phi) S_i^\eta + \sin(\mathbf{Q} \cdot \mathbf{r}_i + \phi) S_i^\xi, \quad (4b)$$

$$S_i^z = -S_i^\xi. \quad (4c)$$

Here $\mathbf{Q}$ is the wave vector and ϕ the phase of the helix. The transformation to bosons is

$$S_i^\xi + iS_i^\eta = \sqrt{2S} [1 - a_i^+ a_i / (2S)] a_i, \quad (5a)$$

$$S_i^x - iS_i^y = \sqrt{2S} a_i^+, \quad (5b)$$

$$S_i^z = S - a_i^+ a_i. \quad (5c)$$

The classical state is obtained by setting $a_i = a_i^+ = 0$. In terms of the Fourier transformed boson operators the exchange Hamiltonian is

$$\begin{aligned}
\mathcal{H}_{Ex} = & E_0(\mathbf{Q}) + \sum_{\mathbf{k}} A_{\mathbf{k}} a_{\mathbf{k}}^+ a_{\mathbf{k}} + \frac{1}{2} \sum_{\mathbf{k}} B_{\mathbf{k}} (a_{\mathbf{k}}^+ a_{-\mathbf{k}}^+ + a_{\mathbf{k}} a_{-\mathbf{k}}) \\
& - \frac{1}{\sqrt{2NS}} \sum_{1,2,3} \frac{1}{2} (C_2 + C_3) \delta(1-2-3) (a_1^+ a_2 a_3 + a_2^+ a_3^+ a_1) + \frac{1}{2NS} \sum_{1,2,3,4} V_{123} \delta(1+2-3-4) a_1^+ a_2^+ a_3 a_4 \\
& - \frac{1}{2NS} \sum_{1,2,3,4} \frac{1}{3} (B_2 + B_3 + B_4) \delta(1-2-3-4) a_1^+ a_2 a_3 a_4 \\
& + \left(\frac{1}{2NS} \right)^{3/2} \sum_{1,2,3,4,5} C_{1-3} \delta(1+2-3-4-5) a_1^+ a_2^+ a_3 a_4 a_5 \\
& + \left(\frac{1}{2NS} \right)^2 \sum_{1,2,3,4,5,6} \frac{1}{2} B_{1-5-6} \delta(1+2-3-4-5-6) a_1^+ a_2^+ a_3 a_4 a_5 a_6,
\end{aligned} \quad (6)$$

where $1 \equiv \mathbf{k}_1$, $2 \equiv \mathbf{k}_2$, etc., $E_0(\mathbf{Q}) = -NJ(\mathbf{Q})S^2$, and

$$2A_{\mathbf{k}} = 4J(\mathbf{Q}) - 2J(\mathbf{k}) - J(\mathbf{Q} + \mathbf{k}) - J(\mathbf{Q} - \mathbf{k}), \quad (7a)$$

$$2B_{\mathbf{k}} = J(\mathbf{Q} + \mathbf{k}) + J(\mathbf{Q} - \mathbf{k}) - 2J(\mathbf{k}), \quad (7b)$$

$$C_{\mathbf{k}} = J(\mathbf{Q} - \mathbf{k}) - J(\mathbf{Q} + \mathbf{k}), \quad (7c)$$

$$2V_{123} = D_{1-3} + D_{2-3} - A_1 - A_2, \quad (7d)$$

$$D_{\mathbf{k}} = 2J(\mathbf{Q}) - J(\mathbf{Q} + \mathbf{k}) - J(\mathbf{Q} - \mathbf{k}), \quad (7e)$$

where $J(\mathbf{k}) = \sum_j J_{ij} \cos(\mathbf{k} \cdot \mathbf{r}_{ij})$. The value of $\mathbf{Q}$ is found by minimizing the free energy with respect to $\mathbf{Q}$, so that $\mathbf{Q} = \mathbf{Q}(j_2, j_3)$. It is simpler, however, to formulate the discussion in terms of $\mathbf{Q}$, j_2 , and j_3 leaving $\mathbf{Q}$ as an implicit function of j_2 and j_3 .

The Zeeman Hamiltonian H_Z is $V(h) \equiv \frac{1}{2} h [e^{i\phi} + e^{-i\phi} V_-]$, where

$$\begin{aligned}
V_{\pm} = & \sqrt{2NS} (a_{\mp\mathbf{Q}}^+ - a_{\mp\mathbf{Q}}) + 2 \sum_{\lambda} a_{\mp\mathbf{Q}+\lambda}^+ a_{\lambda} \\
& \pm \frac{1}{\sqrt{2NS}} \sum_{\lambda\tau} a_{\mp\mathbf{Q}+\lambda}^+ a_{\lambda} a_{\tau}
\end{aligned} \quad (8)$$

One needs the transformation to normal modes

$$a_{\mathbf{k}}^+ = l_{\mathbf{k}} \alpha_{\mathbf{k}}^+ + m_{\mathbf{k}} \alpha_{-\mathbf{k}}, \quad (9)$$

where

$$l_{\mathbf{k}} = \left(\frac{A_{\mathbf{k}} + E(\mathbf{k})}{2E(\mathbf{k})} \right)^{1/2}, \quad (10a)$$

$$m_{\mathbf{k}} = -\frac{B_{\mathbf{k}}}{|B_{\mathbf{k}}|} \left(\frac{A_{\mathbf{k}} - E(\mathbf{k})}{2E(\mathbf{k})} \right)^{1/2}, \quad (10b)$$

where $E(\mathbf{k}) = (A_{\mathbf{k}}^2 - B_{\mathbf{k}}^2)^{1/2}$ in terms of which the quadratic part of $\mathcal{H}_{Ex}$ is

$$\mathcal{H}_0 = S \sum_{\mathbf{k}} E_{\mathbf{k}} \alpha_{\mathbf{k}}^+ \alpha_{\mathbf{k}} + \text{const}, \quad (11)$$

where the constant (the zero-point energy) is not needed here. One can write $\mathcal{H}$ in terms of normal mode operators. The result will involve terms linear in $\alpha_{\mathbf{k}}^+$ (and $\alpha_{\mathbf{k}}$). These terms can be eliminated by setting

$$\alpha_{\mathbf{k}}^+ = \tilde{\alpha}_{\mathbf{k}}^+ + \alpha_{\mathbf{k}}^{+(0)}, \quad \alpha_{\mathbf{k}} = \tilde{\alpha}_{\mathbf{k}} + \alpha_{\mathbf{k}}^{(0)}, \quad (12)$$

where the constants $\alpha_{\mathbf{k}}^{(0)}$ and $\alpha_{\mathbf{k}}^{+(0)}$ represent distortions in the spins orientations induced by the external field. Note that in general $\alpha_{\mathbf{k}}^{+(0)} \neq (\alpha_{\mathbf{k}}^{(0)})^*$ because $\mathcal{H}$ is non-Hermitian. Up to order $\hbar^2$ and to leading order in $1/S$ we find that⁹

$$\begin{aligned}
(\tilde{\alpha}_{\mathbf{k}}^{+(0)})^* = & \alpha_{\mathbf{k}}^{(0)} \\
= & \frac{\hbar}{4} \sqrt{\frac{2N}{S}} \frac{l_{\mathbf{Q}} - m_{\mathbf{Q}}}{E_{\mathbf{Q}}} (-e^{i\phi} \delta_{\mathbf{k}, \mathbf{Q}} + e^{-i\phi} \delta_{\mathbf{k}, -\mathbf{Q}}) \\
& - \frac{\hbar^2 (2N)^{1/2}}{16 (S^3)} \frac{(l_{\mathbf{Q}} - m_{\mathbf{Q}})^2}{E_{\mathbf{Q}}} \frac{(l_{2\mathbf{Q}} - m_{2\mathbf{Q}})}{E_{2\mathbf{Q}}} \\
& \times \Delta_{\mathbf{Q}} (e^{2i\phi} \delta_{\mathbf{k}, 2\mathbf{Q}} - e^{-2i\phi} \delta_{\mathbf{k}, -2\mathbf{Q}}),
\end{aligned} \quad (13)$$

where $\Delta_{\mathbf{Q}}$ is unity for $3\mathbf{Q} = \mathbf{G}$, which is the only case of present interest. This evaluation yields the $\hbar$ -dependent energy at $T = 0$ as

$$\begin{aligned}
E(h) - E(h=0) = & -\frac{1}{4} N \hbar^2 [2J(\mathbf{Q}) - J(2\mathbf{Q}) - J(0)]^{-1} \\
& + \left(\frac{N \hbar^3}{S} \right) \cos 3\phi \sum_{\mathbf{G}} \delta_{3\mathbf{Q}, \mathbf{G}} + O(\hbar^4).
\end{aligned} \quad (14)$$

To leading order in $1/S$, $\Gamma = 0$, in agreement with the $T=0$ evaluation of the previous result⁶ for the classical ($S \rightarrow \infty$) model. The new result is that to next order in $1/S$, $\Gamma \neq 0$.

For such a calculation one must consider the effect of perturbations generated following the transformation of Eq. (12). The relevant perturbations are

$$V_A = \hbar e^{i\phi} \sum_{\mathbf{k}} V_A(\mathbf{k}) \tilde{\alpha}_{\mathbf{k}+\mathbf{Q}}^+ \tilde{\alpha}_{\mathbf{k}} + \cdots, \quad (15a)$$

$$V_B = \hbar^2 S^{-1} e^{2i\phi} \sum_{\mathbf{k}} V_B(\mathbf{Q}) \tilde{\alpha}_{\mathbf{k}+2\mathbf{Q}}^+ \tilde{\alpha}_{\mathbf{k}} + \cdots, \quad (15b)$$

$$V_C = \hbar^3 S^{-2} e^{3i\phi} \sum_{\mathbf{k}} V_C(\mathbf{k}) \tilde{\alpha}_{\mathbf{k}+3\mathbf{Q}}^+ \tilde{\alpha}_{\mathbf{k}} + \cdots, \quad (15c)$$

where the ellipses indicate the three other terms with coefficients similar to $V_A(\mathbf{k})$, $V_B(\mathbf{k})$, and $V_C(\mathbf{k})$ that one gets when each $\tilde{\alpha}_{\mathbf{k}}^+$ and $\tilde{\alpha}_{-\mathbf{k}}$ is replaced, respectively, by $\tilde{\alpha}_{-\mathbf{k}}$ and $\tilde{\alpha}_{\mathbf{k}}^+$. All the coefficients in Eqs. (15) are defined to be independent of S .

Contributions to Γ of order $1/S$ (for $p=3$) come from terms in perturbation theory due to V_A , V_B , and V_C which

contribute to order h^3 . Perturbation of higher order in $1S$ than those of Eq. (15) do not contribute to Γ at order $1/S$. Due to space limitations I only quote the final result:

$$\begin{aligned}
256S\Delta^3\Gamma = & \frac{8}{N} \sum_k \frac{(c_{k+Q} - c_k)(c_{k-Q} - c_{k+Q})}{(E_k + E_{k-Q})(E_k + E_{k+Q})} (c_k - c_{k-Q})(l_{k+Q} - m_{k+Q})^2 (l_k - m_k)^2 (l_{k+Q} - m_{k+Q})^2 \\
& + 8 \sum_k l_k m_k (\Delta + 3c_{Q+k} + a_k + a_Q - 2a_{k+Q} + 2b_{k+Q} - 2b_k) - 8 \sum_k m_k^2 (2\Delta + 4c_{Q+k} - b_k + 2a_k \\
& + 2a_Q - 2a_{k-Q} + 2b_{k+Q}) - 4 \sum_k \frac{c_{k+Q} - c_k}{E_k + E_{k+Q}} (l_{k+Q} - m_{k+Q})^2 (l_k - m_k)^2 (c_{k+Q} - c_k + 2\Delta - 3a_k \\
& + 4a_{k-Q} \\
& - 4b_{k-Q} - b_{k+Q}) + 2 \sum_k \frac{c_{k+Q} - c_k}{E_k E_{k+Q}} (8\Delta + 4b_k - a_k - a_{k+Q} + 2b_{k+Q}), \quad (16)
\end{aligned}$$

where $\Delta \equiv J(Q) - J(0)$.

As it stands this result is not very informative. We would like to know whether or not Γ vanishes. For this purpose we consider a generalization of this model in which the couplings in the a - b plane are unchanged, but now we couple not just into a third direction but into d transverse directions, such that all interactions between nearest neighbors in each of these d directions is described by an exchange integral J_1 that is much larger than $j_1=1$, j_2 , and j_3 . In that limit it is useful to write $\mathbf{k} = k_x \hat{i} + k_y \hat{j} + \mathbf{k}_\perp$, where $\mathbf{k}_\perp$ is perpendicular to the x - y plane. Looking back at Eqs. (7), we see that B_k and C_k are independent of J_1 and $\mathbf{k}_\perp$, for instance. Likewise we can write

$$2A_k = 4[J_1(0) - J_1(\mathbf{k}_\perp)] + 2a_k, \quad (17)$$

where a_k is the value of A_k when J_1 is zero and is thus independent of $\mathbf{k}_\perp$. In this way one can develop a systematic expansion in j/J_1 . The result to lowest order in this parameter is

$$\Gamma = \frac{|j|^2}{8NS\Delta^3} \sum_k \frac{1}{J_1(0) - J_1(\mathbf{k})}, \quad (18)$$

where $|j|^2 \equiv 4(j_1^2 + j_2^2 + j_3^2)$. We therefore conclude that in general Γ is nonzero at order $1/S$. This result is quite

reasonable: If one believes that quantum fluctuations are similar in effect to thermal fluctuations, one would indeed expect Γ to be nonzero. We refer the reader to an earlier paper⁶ for a discussion of some of the experimental consequences of this nonzero pinning energy.

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