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**Abstract**

The commensurability energy $\Delta E$ 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**

Physics | Quantum Physics

# Phase locking in the Heisenberg helimagnet

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The commensurability energy $\Delta E$ 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 is[1]

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

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

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 $\epsilon$ 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 $J_{ij}\equiv J(\mathbf{r}_i - \mathbf{r}_j)$ 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, $J_{ij}=J_\perp>0$. All other interactions are neglected. For sufficiently negative values of $j_2$ and/or $j_3$ the classical ground state of this model is[1] 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 calculations[3–5] 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 shown[6] that nonlinear spin-wave interactions modified this picture. For small $h$ the pinning free energy (omitted in the early work) is of the form

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

where $p$ is an integer, $\mathbf{G}$ a (big) reciprocal lattice vector, and $\phi$ the phase of the helix. Minimization with respect to $\phi$ 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] Previously[6] 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 Lange[4] 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

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

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

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

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

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

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

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

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

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

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 $J(\mathbf{k})=\Sigma_j J_{ij}\cos(\mathbf{k}\cdot\mathbf{r}_{ij})$. 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 $V(h)\equiv\frac{1}{4}h[e^{i\phi}+e^{-i\phi}V_-]$, where

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

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 $\mathscr{H}_{Ex}$ is

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

where the constant (the zero-point energy) is not needed here. One can write $\mathscr{H}$ 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

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

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 $\alpha_{\mathbf{k}}^{+(0)}\neq(\alpha_k^{(0)})^*$ because $\mathscr{H}$ is non-Hermitian. Up to order $h^2$ and to leading order in $1/S$ we find that[9]

$$(\alpha_{\mathbf{k}}^{+(0)})^*=\alpha_{\mathbf{k}}^{(0)}$$
$$=\frac{h}{4}\sqrt{\frac{2N}{S}}\frac{l_{\mathbf{Q}}-m_{\mathbf{Q}}}{E_{\mathbf{Q}}}(-e^{i\phi}\delta_{\mathbf{k},\mathbf{Q}}+e^{-i\phi}\delta_{\mathbf{k},-\mathbf{Q}})$$
$$-\frac{h^2}{16}\left(\frac{2N}{S^3}\right)^{1/2}\frac{(l_{\mathbf{Q}}-m_{\mathbf{Q}})^2}{E_{\mathbf{Q}}}\frac{(l_{2\mathbf{Q}}-m_{2\mathbf{Q}})}{E_{2\mathbf{Q}}}$$
$$\times\Delta_{\mathbf{Q}}(e^{2i\phi}\delta_{\mathbf{k},2\mathbf{Q}}-e^{-2i\phi}\delta_{\mathbf{k},-2\mathbf{Q}}), \quad (13)$$

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

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

To leading order in $1/S$, $\Gamma=0$, in agreement with the $T=0$ evaluation of the previous result[6] for the classical ($S\to\infty$) 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

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

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

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

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 $\Gamma$ 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 $\Gamma$ at order $1/S$. Due to space limitations I only quote the final result:

$$256S\Delta^3\Gamma=\frac{8}{N}\sum_{\mathbf{k}}\frac{(c_{\mathbf{k}+\mathbf{Q}}-c_{\mathbf{k}})(c_{\mathbf{k}-\mathbf{Q}}-c_{\mathbf{k}+\mathbf{Q}})}{(E_{\mathbf{k}}+E_{\mathbf{k}-\mathbf{Q}})(E_{\mathbf{k}}+E_{\mathbf{k}+\mathbf{Q}})}(c_{\mathbf{k}}-c_{\mathbf{k}-\mathbf{Q}})(l_{\mathbf{k}+\mathbf{Q}}-m_{\mathbf{k}+\mathbf{Q}})^2(l_{\mathbf{k}}-m_{\mathbf{k}})^2(l_{\mathbf{k}+\mathbf{Q}}-m_{\mathbf{k}+\mathbf{Q}})^2$$
$$+8\sum_{\mathbf{k}}l_{\mathbf{k}}m_{\mathbf{k}}(\Delta+3c_{\mathbf{Q}+\mathbf{k}}+a_{\mathbf{k}}+a_{\mathbf{Q}}-2a_{\mathbf{k}+\mathbf{Q}}+2b_{\mathbf{k}+\mathbf{Q}}-2b_{\mathbf{k}})-8\sum_{\mathbf{k}}m_{\mathbf{k}}^2(2\Delta+4c_{\mathbf{Q}+\mathbf{k}}-b_{\mathbf{k}}+2a_{\mathbf{k}}$$
$$+2a_{\mathbf{Q}}-2a_{\mathbf{k}-\mathbf{Q}}+2b_{\mathbf{k}+\mathbf{Q}})-4\sum_{\mathbf{k}}\frac{c_{\mathbf{k}+\mathbf{Q}}-c_{\mathbf{k}}}{E_{\mathbf{k}}+E_{\mathbf{k}+\mathbf{Q}}}(l_{\mathbf{k}+\mathbf{Q}}-m_{\mathbf{k}+\mathbf{Q}})^2(l_{\mathbf{k}}-m_{\mathbf{k}})^2(c_{\mathbf{k}+\mathbf{Q}}-c_{\mathbf{k}}+2\Delta-3a_{\mathbf{k}}$$
$$+4a_{\mathbf{k}-\mathbf{Q}}$$
$$-4b_{\mathbf{k}-\mathbf{Q}}-b_{\mathbf{k}+\mathbf{Q}})+2\sum_{\mathbf{k}}\frac{c_{\mathbf{k}+\mathbf{Q}}-c_{\mathbf{k}}}{E_{\mathbf{k}}E_{\mathbf{k}+\mathbf{Q}}}(8\Delta+4b_{\mathbf{k}}-a_{\mathbf{k}}-a_{\mathbf{k}+\mathbf{Q}}+2b_{\mathbf{k}+\mathbf{Q}}), \tag{16}$$

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

As it stands this result is not very informative. We would like to know whether or not $\Gamma$ 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 $J_\perp$ 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 $B_{\mathbf{k}}$ and $C_{\mathbf{k}}$ are independent of $J_\perp$ and $\mathbf{k}_\perp$, for instance. Likewise we can write

$$2A_{\mathbf{k}}=4[J_\perp(0)-J_\perp(\mathbf{k}_\perp)]+2a_{\mathbf{k}}, \tag{17}$$

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

$$\Gamma=\frac{|j^2|}{8NS\Delta^3}\sum_{\mathbf{k}}\frac{1}{J_\perp(0)-J_\perp(\mathbf{k})}, \tag{18}$$

where $|j|^2\equiv4(j_1^2+j_2^2+j_3^2)$. We therefore conclude that in general $\Gamma$ 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 $\Gamma$ to be nonzero. We refer the reader to an earlier paper[6] for a discussion of some of the experimental consequences of this nonzero pinning energy.

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[9] Within spin-wave theory (i.e., avoiding low-dimensional divergent fluctuations) the response obtained from Eq. (13) is finite. The observable angular displacement is proportional to $a_{\mathbf{Q}}^{(0)}\equiv l_{\mathbf{Q}}\alpha_{\mathbf{Q}}^{(0)}-m_{\mathbf{Q}}\alpha_{\mathbf{Q}}^{+(0)}$. This quantity is of order $(l_{\mathbf{Q}}-m_{\mathbf{Q}})^2/E_{\mathbf{Q}}$ but remains finite even though $E_{\mathbf{Q}}=0$. To see this use Eq. (10), nothing that $B_{\mathbf{Q}}<0$ and $A_{\mathbf{Q}}$ is nonzero. Then for $\mathbf{k}$ near $\mathbf{Q}$, Eq. (10) yields $l_{\mathbf{k}}-m_{\mathbf{k}}\sim\sqrt{E_{\mathbf{k}}}$ for small $E_{\mathbf{k}}$.