LA-UR- 86-2887

TITLE: THERMOMAGNETIC TRANSPORT COEFFICIENTS: SOLITONS IN AN EASY PLANE MAGNETIC CHAIN

AUTHOR(S): G. M. Wysin
P. Kumar

SUBMITTED TO: Physical Review B

Phys. Rev. B 36, 7063 (1987)

Los Alamos

Los Alamos National Laboratory
Los Alamos, New Mexico 87545

Thermomagnetic Transport Coefficients: Solitons in an Easy Plane Magnetic Chain

G. M. Wysin* and P. Kumar
Department of Physics
University of Florida
Gainesville, FL 32611

Abstract

Using a simple model, we calculate the transport properties of a one-dimensional easy-plane ferromagnet in the presence of an in-plane magnetic field. The model incorporates the combined effects of a magnetic field gradient and a temperature gradient acting on a gas of solitons and spin waves. Suggestions are made for experiments capable of measuring these effects in materials such as $CsNiF_3$ and CHAB [$(C_6H_{11}NH_3)CuBr_3$]. We also discuss their use as another type of probe for solitons.

PACS Cat. no. 75.10.Jm, 66.70.+f, 05.60.+w

I. Introduction

Long range order cannot exist in one dimension (1-D), however short range order is possible. For the particular case of one dimensional magnets,[1,2] the spins interact largely along a specific chain direction. The interaction between the chains is weak and leads to three dimensional ordering at some low temperature T_c. For $T \gtrsim T_c$, there is a wide range of temperature (depending on the ratio of in-chain and interchain exchange constants) where spins display short-range order along the chains. The ordered regions are separated by domain walls. These walls are dynamic objects and in an easy plane system, their properties are similar to those of sine Gordon (sG) solitons. The thermodynamics above T_c is then determined by the linear waves (magnons) and solitons.[3] An extensive series of neutron scattering, susceptibility, specific heat and spin relaxation measurements lend qualitative, occasionally even quantitative, support to this picture, for materials such as $CsNiF_3$[1] and CHAB $[(C_6H_{11}NH_3)CuBr_3]$,[4] and also for antiferromagnets such as TMMC $[(CD_3)_4NMnCl_3]$.[2]

The object here is to investigate whether the waves and soliton picture from equilibrium thermodynamics can be extended to transport phenomena, in terms of weakly coupled soliton and magnon ideal gases, subjected to gradients of temperature and applied field. Also, we look into the possibility of analogues of two well known effects in semiconductors (where the carriers are described semiclassically). In a semiconductor, carriers can be moved by application of either an electric field or a temperature gradient. Application of one of them leads to, under proper circuit conditions, appearance of the other. The equivalent quantities here are the magnetic field gradient and the temperature gradient. The former changes directly the energy of the soliton while the latter affects the thermal population. Thus a field gradient can cause the soliton (or magnon) population to increase at one end of the sample, leading to an effective increase in temperature and vice versa. In as much as an easy plane ferromagnetic chain can be described by sine Gordon theory, and that an ideal gas-like description of the sG model is feasible, it should be possible to study this and other transport effects in a 1-D magnetic system.

The calculations described below are in the ideal gas view of thermodynamics. An obvious improvement of this work will be to address the well known difficulties (quantum spins and excursions off the easy plane) of the sG description, and include more precisely the interactions between solitons and between solitons and magnons. Here the effects of the magnons upon the solitons are grossly taken into account via an appropriate normalization of the equilibrium soliton distribution function f^0, as taken from Ref. 3 (CKBT). We calculate the magnon response treating them as a degenerate boson gas while keeping the solitons non-degenerate. We have also assumed a single relaxation time. Again, in semiconductors, the relaxation times for mass/charge current and the heat current are different. We expect the relaxation times for mass and heat currents of solitons to be different as well. Yet, we expect the calculations reported below to be qualitatively correct. Indeed an experiment would provide invaluable help in constructing transport theory of nonlinear excitations.

II. Transport Formalism

The ferromagnetic Hamiltonian for the spin degrees of freedom of a single chain is taken to be[5]

$$H = \sum_{n=1}^{N} [-J\, \vec{S}_n \cdot \vec{S}_{n+1} + A(S_n^z)^2 - HS_n^x] \quad . \tag{1}$$

Here J is the nearest neighbor exchange coupling, $A > 0$ is the single ion anisotropy, the $\vec{S}_n$ are classical spin vectors, and the applied field H ($= g\mu_B B$) is in the easy (xy) plane; g and μ_B are the Lande g-factor and Bohr magneton respectively. Using spherical coordinates $\vec{S}_n$ = S ($\cos\theta \cos\phi$, $\cos\theta \sin\phi$, $\sin\theta$), and assuming $H/2AS \ll 1$, a continuum limit approximately produces a sine-Gordon equation of motion for the in-plane angle ϕ:

$$c_0^2 \phi_{zz} - \phi_{tt} = \omega_0^2 \sin\phi \quad , \quad \theta = (\hbar/2AS)\phi_t \tag{2a}$$

with

$$c_0^2 = 2AJS^2a^2/\hbar^2 \quad , \quad \omega_0^2 = 2AHS/\hbar^2 \quad , \tag{2b}$$

where a is the lattice spacing and z is the position on the chain. This sG limit has essentially converted the out-of-plane degree of freedom θ to the momentum conjugate to ϕ -- this linearization of a nonlinear degree of freedom is a substantial part of the error introduced in approximating the full equations of motion by a sG equation. The sG equation has well-known soliton, breather, and low amplitude linear modes, and we review some of their properties needed here.[6]

The solitons are traveling wave rotations of the spins through 2π within the easy plane, with the spin-tilting out of the easy plane being proportional to the soliton velocity $v < c_0$. This rotation occurs over a characteristic length d_0, determined by the applied field (for velocities $v \ll c_0$)

$$d_0 = c_0/\omega_0 = \sqrt{JS/H} \quad . \tag{3}$$

The energy is that of a relativistic particle of rest mass m_0, and rest energy E_0,

$$E = E_0\gamma \quad , \quad \gamma = (1-v^2/c_0^2)^{-1/2} \quad , \tag{4a}$$

$$E_0 = 8(JHS^3)^{1/2} \quad , \quad m_0 = E_0/c_0^2 \quad , \tag{4b}$$

but for simplicity we shall use the nonrelativistic limit for γ, $\gamma = 1 + \frac{1}{2}(v^2/c_0^2)$. The solitons will be treated using classical Maxwell-Boltzman statistics.

The dispersion relation for the linear modes, or magnons in the present context, as a function of wavevector k is

$$\varepsilon_k^2 = \varepsilon_0^2 + (\hbar c_0 k)^2 \quad , \tag{5a}$$

$$\varepsilon_0 = \hbar\omega_0 = \frac{1}{8S} \; \alpha \; E_0 \quad , \quad \alpha \equiv \frac{2A}{J} \quad . \tag{5b}$$

The relative anisotropy $2A/J \simeq .38$ for spin-1 $CsNiF_3$;[7] so typically the energy gap for magnons is much smaller than for the solitons ($\varepsilon_0/E_0 \simeq .07$). The magnons will be treated using Bose-Einstein statistics.

Breather states are bound soliton-antisoliton pairs with an internal frequency. Their contributions are neglected in this calculation. The low energy breathers can be thought of as bound magnon states, dependent on the interaction between magnons, and as such represent a correction term to the soliton-magnon ideal gas theory. In the simplest equilibrium thermodynamics theory their effects can be neglected. Similarly, we expect that the neglect of breathers in this transport calculation introduces relatively small errors, especially in a paramter regime where solitons are important.

The model used here to calculate the transport properties of this easy plane ferromagnetic chain consists of a two-component ideal gas of magnons and solitons. Any interaction between magnons and solitons leads to (a) normalization of their energies and (b) a relaxation time τ representing approach to equilibrium. This picture is exact within sG theory which is completely integrable. If we stay close to the field and temperature region where the sG picture is approximately valid, we are allowed to assume that the interaction corrections are negligible. More precisely, we assume that the approach to equilibrium is caused by an extrinsic mechanism, e.g. magneto-elastic coupling leading to scattering of magnons and solitons by phonons. The intrinsic relaxation rate for scattering of solitons by magnons is assumed to be negligible as compared to the extrinsic relaxation ratio. This also means that a Matthiessen's type rule exists namely, the soliton and magnon transport currents are additive. In the following the soliton and magnon currents are calculated separately.

The nonequilibrium thermodynamics of both solitons and magnons is described by a linearized Boltzman equation. In a steady state, the change in distribution function $\delta f(z,p)$ from its equilibrium value $f^0(z,p)$ satisfies (in the relaxation time approximation),

$$- \frac{\delta f}{\tau} = \frac{\partial E}{\partial p} \cdot \frac{\partial f^0}{\partial z} + F \cdot \frac{\partial f^0}{\partial p} \tag{6}$$

where $E(z,p)$ is the energy of the carriers, dependent on position due to the applied temperature and field gradients, and dependent on momentum p. The applied force F represents the effect of the field gradient.

In principle equation (6) should be derived from a microscopic field theory of the Hamiltonian in equation (1). Such a derivation is beyond the scope of this paper. One expects that such a calculation will lead to a Boltzmann equation with terms corresponding individually to renormalized solitons and magnons together with relatively small interaction terms, accounting for soliton-soliton, soliton-magnon, and magnon-magnon (or also breathers) interactions. As a lowest order calculation we presently ignore these interaction terms, except for the modification of the soliton equilibrium distribution by the magnons. (See section IIA). Then, with this approximation, the soliton and magnons are effectively treated as independent ideal gases. This simplified calculation offers a much clearer view of the kinetic physical processes involved, avoiding the mathematical difficulties, at the expense of some accuracy. These higher order interaction effects are known to improve agreement between theory and experiment for some equilibrium properties (e.g. specific heat peaks of $CsNiF_3$ and CHAB), but principally only by rescaling various parameters while leaving the functional form intact.[8] We might expect similar behavior for the transport properties.

The effect of the field gradient will be treated as follows. We assume that the length scale $\ell_H \simeq H/(\partial H/\partial z)$ over which the field changes is very large compared to the soliton width d_0. Generally d_0 may be anywhere from a few to tens of lattice spacings, while the field gradient length scale ℓ_B is macroscopic, making this assumption very easily satisfied. Locally, then, the sG solitons are adequate solutions to the equations of motion. But as they move in the slowly changing field, they experience its effect as a mild force towards the region of lower soliton energy (which is towards the lower field region), being adiabatically modified and exchanging energy with the applied field. Thus the force F_s on a soliton is taken to be

$$F_s = -\frac{\partial E}{\partial z} = -\frac{\partial E}{\partial H}\frac{\partial H}{\partial z} = \frac{1}{2}E(-\frac{\nabla H}{H}) \quad . \tag{7}$$

Similarly, the force on a magnon of wavevector k is taken to be

$$F_k = -\frac{\partial E_k}{\partial z} = \frac{\varepsilon_0^2}{2\varepsilon_k}(\frac{-\nabla H}{H}) \quad . \tag{8}$$

In the semiconductor context the physically observable transported quantities are the charge current and heat current. For this magnetic chain, the solitons and magnons similarly carry heat current, but the closest analogue to the charge current is a magnetization current. In particular, there will be only an x-component of magnetization current (parallel to the field); the y and z components average out to zero for both solitons and magnons. Below we treat the different transport properties of solitons and magnons separately.

IIA. Solitons

The magnetization current j_m and heat current j_u will be given by integrals of contributions from solitons of all velocities (less than c_0), over the distribution which has been perturbed from equilibrium by the applied driving "forces",

$$j_m = \int dv\ v\ m(v)\ \delta f(v) \quad , \tag{9a}$$

$$j_u = \int dv\ v\ u(v)\ \delta f(v) \quad . \tag{9b}$$

Here $v = \partial E/\partial p$ represents the velocity; we consider δf as a function of velocity instead of momentum. The functions m(v) and u(v) represent the effective magnetization and "heat" or internal energy carried by a soliton or antisoliton of velocity v. These functions are determined by requiring that the equilibrium magnetization M and internal energy U due to the solitons, as given in Ref. 3, can also be written as integrals over the equilibrium distribution $f^0(v)$;

$$M = \int dv\ m(v)\ f^0(v) \quad , \tag{10a}$$

$$U = \int dv\ u(v)\ f^0(v) \quad . \tag{10b}$$

M and U are given from the soliton/antisoliton equilibrium free energy F_0^{sol}

$$F_0^{sol} = -kT\ n^{tot} \quad , \tag{11a}$$

$$M = -\frac{\partial F_0^{sol}}{\partial H} \quad , \quad U = \frac{\partial}{\partial \beta}(\beta F_0^{sol}) \quad , \tag{11b}$$

where $\beta = (kT)^{-1}$. The total number density of solitons and antisolitons, n^{tot}, is

$$n^{tot} = \frac{4}{d_0}\left(\frac{\beta E_0}{2\pi}\right)^{1/2} e^{-\beta E_0} \quad , \tag{12}$$

with d_0 and E_0 as defined in equations (3) and (4). Certainly integration over $f^0(v)$ should give the total number density of solitons and antisolitons:

$$n^{tot} = \int dv\ f^0(v) \quad . \tag{13}$$

Combining the different expressions for M and U, equations (10) and (11), results in consistency conditions involving m(v), u(v) and $f^0(v)$,

$$kT \frac{\partial f^0}{\partial H} = m(v)\ f^0(v) \quad , \tag{14a}$$

$$\frac{\partial f^0}{\partial \beta} = -u(v)\ f^0(v) \quad . \tag{14b}$$

To completely determine m(v) and u(v) we need to specify $f^0(v)$. Because we assume the solitons obey classical statistics, f^0 can be written as

$$f^0(v) = \frac{A_0}{c_0 d_0}\, e^{-\beta(E-\mu)} \quad , \tag{15}$$

where the factor $c_0 d_0$ gives the correct dimensions, A_0 is a dimensionless constant, and a chemical potential μ has been introduced in order to write f^0 in a standard form. The constant A_0 is required for proper phase space counting; the phase space integral is normalized by Plank's constant, 1/h, $\int dp/h \rightarrow \int dv(m_0/h)$, and thus A_0 is set by

$$\frac{A_0}{c_0 d_0} = \frac{m_0}{h} \quad . \tag{16}$$

With this assumed form for $f^0(v)$, equations (12) and (13) determine the chemical potential μ necessary to recover the CKBT result for total soliton number density (also assuming nonrelativistic dispersion $E = E_0 + \frac{1}{2} m_0 v^2$);

$$\mu = \frac{1}{\beta}\, \ell n\left(\frac{2\beta E_0}{\pi A_0}\right) \quad , \tag{17}$$

and thus $f^0(v)$ has been specified.

Some comments are in order related to the chemical potential. The quantity μ appears explicitly in Eq. (15) as a chemical potential, and indeed will appear in the Boltzmann equation again as a chemical potential (Eq. 23). Effectively the factor $e^{\beta\mu}$ provides the appropriate normalization for f^0, such that we can reproduce the CKBT results for n^{tot}, M, U, and so on, while at the same time putting f^0 in a familiar standard form.

If μ is taken to represent a real effective chemical potential, then it is interesting to consider its effects on quantum degeneracy. Typically quantum degeneracy is expected to become important when μ passes through zero, thereby implying that each soliton is confined to an area approaching h or less in phase space. Equation (17) then gives a corresponding degeneracy temperature T_q defined by

$$kT_q = 4\hbar\omega_0 = \frac{\alpha^{1/2}}{2S} E_0 \quad . \tag{18}$$

One finds $kT_q \simeq \frac{3}{10} E_0$ for either $CsNiF_3$ or CHAB, i.e., rather larger than expected when compared to E_0. However, one of the assumptions of the classical ideal gas soliton thermodynamics[3] is that $kT \ll E_0$, and we see that there appears to be a limited range of temperatures over which the classical approach will be valid. Usually one would attempt to correct this situation by considering the quantum corrections for the statistical mechanics of the sG equation. This viewpoint will not be adopted here. Instead, we recall that the classical sine-Gordon thermodynamics does remarkably well in describing equilibrium experimental data for both $CsNiF_3$ and CHAB, even for temperatures well below the predicted T_q (for instance, as low as $kT_q \simeq \frac{1}{4}E_0$). In view of such experimental evidence available, it seems reasonable to attempt to use the same classical sG thermodynamics also to describe transport in these easy-plane ferromagnets, and for the present to ignore any difficulties which may be implied by the relatively high T_q. And, of course, it is not clear whether we can really treat μ as a true chemical potential anyway. Indeed, the locations of the quantum and classical regimes for these materials, for both equilibrium and nonequilibrium problems, is an issue yet to be resolved.

Then, with $f^0(v)$ as already specified, the consistency conditions (14) determine m(v) and u(v) as

$$m(v) = -\frac{\partial}{\partial H}(E-\mu) + \frac{1}{2}kT/H = -(\tfrac{1}{2}E-kT)/H \quad , \tag{19a}$$

$$u(v) = \frac{\partial}{\partial \beta}[\beta(E-\mu)] = E-kT \quad . \tag{19b}$$

It can be easily verified that these reproduce the known low temperature limit $\beta E_0 > 1$ equilibrium quantities,

$$M^{sol} = -\frac{1}{2}n^{tot}(E_0 - \tfrac{3}{2}kT)/H \quad , \tag{20a}$$

$$U^{sol} = n^{tot}(E_0-\tfrac{1}{2}kT) \quad . \tag{20b}$$

It should be mentioned that m(v) and u(v) include the leading order effects of the linear modes acting on the solitons, as obtained in equilibrium. The number density used here includes the self energy effects of scattering events of the linear modes with the solitons. To see this in a different manner, consider the magnetization pulse carried by a single unperturbed moving sG soliton. The x-component of the soliton profile is a pulse deviating from the aligned ground state, with characteristic width d_0/γ,

$$S^x = S(1-2\ \mathrm{sech}^2 \gamma z/d_0) \quad . \tag{21}$$

Relative to the ground state, the total x-magnetization carried is

$$\tilde{m}^x = \int_{-\infty}^{\infty} dz(S^x - S) = -4Sd_0/\gamma \quad . \tag{22}$$

This result shows that for faster moving solitons, which get narrower due to the relativistic contraction, the absolute value of the magnetization carried decreases with increasing velocity. This is in contrast to the previous result for m(v) Eq. 19a, including temperature and linear modes acting on the soliton, where |m(v)| increases with increasing velocity (for $\beta E_0 > 2$). This reflects the effective soliton mass increase induced by the linear modes. In any case integration of $\tilde{m}^x$ over all velocities cannot give the known equilibrium magnetization. This observation originally led to the present self consistent method for determining m(v) and u(v).

To completely specify the currents, we rewrite δf in terms of the applied temperature and field gradients, and the force F,

$$-\delta f/\tau = v\left(\frac{\partial f^0}{\partial E}\right)\{(E-\mu)(-\nabla T/T) - \nabla\mu + F\} \quad . \tag{23}$$

Since μ is a function of T and H, we can eliminate $\nabla\mu$ in favor of ∇T and ∇H,

$$\nabla\mu = (kT-\mu)(-\nabla T/T) - kT(-\nabla H/H) \quad . \tag{24}$$

Thus the soliton transport results are determined only by ∇T and ∇H. Again, using the nonrelativistic energy relationship, we obtain

$$j_u = K_{uT}^{sol}(-\nabla T/T) + K_{uH}^{sol}(-\nabla H/H) \quad , \tag{25a}$$

$$j_m = K_{mT}^{sol}(-\nabla T/T) + K_{mH}^{sol}(-\nabla H/H) \quad , \tag{25b}$$

with transport coefficients

$$K_{uT}^{sol} = a_1 I_0[(\beta E_0)^2 + (\beta E_0) + \tfrac{7}{4}] \quad , K_{uH}^{sol} = a_1 I_0[(\beta E_0)^2 + 4\beta E_0 + \tfrac{13}{4}] \quad , \tag{26a}$$

$$K_{mT}^{sol} = a_2 I_0[(\beta E_0)^2 + \tfrac{5}{4}] \quad , \quad K_{mH}^{sol} = a_2 I_0[(\beta E_0)^2 + 3\beta E_0 - \tfrac{1}{4}] \quad , \tag{26b}$$

where

$$a_1 = \frac{\tau c_0}{\beta^2} \quad , \quad a_2 = -\frac{\tau c_0}{\beta^2} \cdot \frac{1}{2H} \quad , \tag{27a}$$

$$I_0 = \frac{\alpha}{8\pi S^2}^{1/2} (\beta E_0)^{1/2} e^{-\beta E_0} \quad . \tag{27b}$$

Aside from some prefactors these results depend only on βE_0. There is no Onsager symmetry relationship relating K_{mT}^{sol} and K_{uH}^{sol}, due to the fact that the field gradient creates <u>velocity dependent forces</u> (recall $F \sim E$), thereby eliminating any Onsager symmetry. K_{mT}^{sol} and K_{mH}^{sol} are both negative since the soliton magnetization is always a deviation from the aligned ground state configuration.

IIB. Magnons

The general approach used for magnons is the same as for the solitons, with some minor differences. They will be described by Bose-Einstein statistics, with zero chemical potential, and the phase space integrals will be over wave vectors k instead of velocity. Again the presence of velocity dependent forces implies a lack of Onsager symmetry. The magnetization and heat carried by a magnon of wavevector k are

$$m(k) = -\frac{\varepsilon_0^2}{2H\varepsilon_k} \tag{28a}$$

$$u(k) = \varepsilon_k \tag{28b}$$

The equilibrium distribution is assumed to be

$$f_k^0 = \frac{1}{e^{\beta\varepsilon_k}-1} \quad , \tag{29}$$

then we obtain the following magnon transport coefficients

$$K_{uT}^{mag} = a_1\ (\beta\varepsilon_0)^{-1}\ s_2(\beta\varepsilon_0) \quad , \quad K_{uH}^{mag} = a_1\ \tfrac{1}{2}\beta\varepsilon_0\ s_0(\beta\varepsilon_0) \quad , \tag{30a}$$

$$K_{mT}^{mag} = a_2\ \beta\varepsilon_0\ s_0(\beta\varepsilon_0) \quad , \quad K_{mH}^{mag} = a_2\ \tfrac{1}{2}(\beta\varepsilon_0)^3\ s_{-2}(\beta\varepsilon_0) \quad , \tag{30b}$$

with the functions $s_n(x_0)$ defined by the integral

$$s_n(x_0) = \frac{1}{4\pi}\int_{x_0}^{\infty} dx\ x^{n-1}(x^2-x_0^2)^{1/2}/\sinh^2(\tfrac{1}{2}x) \quad . \tag{30c}$$

III. Results

Some typical results for these transport coefficients vs. field at fixed temperature and vs. temperature at fixed field are shown in Fig. 1, for parameters appropriate to $CsNiF_3$.[7] Note that to obtain the overall scale of these curves we would need reasonable estimates of the relaxation times τ_{sol} and τ_{mag}. Also note that these are results for a single chain, and must be multiplied by the chain number density per