JOURNAL DE PHYSIQUE
Colloque C8, Supplément au n° 12, Tome 49, décembre 1988

"PSEUDO $T^{3/2}$" LAW FOR MAGNETIC SURFACES INTERFACES AND SUPERLATTICES

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Abstract. – Classical spin-wave theory predicts that the surface magnetisation $M_S(T)$ decreases with temperature twice as fast as in the bulk. It is shown that this result which contradicts experiment breaks down at temperatures as low as 1 % T_C. The local $M_S(T)$ above these temperatures obeys a "pseudo $T^{3/2}$" law whose prefactor is determined by the local exchange. It is shown that "pseudo $T^{3/2}$" law holds also for magnetic interfaces and superlattices.

The Bloch law for the bulk magnetisation

$$M_B(T) / B_B(0) = 1 - M_B T^{3/2} \qquad (1)$$

holds up to temperatures $T \sim T_C/3$. One of the classical results of surface magnetism [1, 2] is that the Bloch law holds also for the surface magnetisation $M_S(T)$ but with a prefactor $B_S = 2B_B$. Measurements of $M_S(T)$ for ferromagnetic metals using SPLEED [3], Mössbauer spectroscopy [4, 5] and low-energy cascade electrons [6] confirm that M_S obeys a $T^{3/2}$ law but with a prefactor B_S which is different for different surfaces and can be as large as $5.4B_B$ [6].

The classical spin-wave theory thus fails to explain the much faster decrease of $M_S(T)$ observed in metals. This is not surprising since it assumes no changes in the local magnetisation and exchange in the surface region. Neither of these assumptions is valid for metals.

The fundamental theoretical question is, therefore, whether a softening of surface exchange or change of magnetisation near the surface can explain the observed large B_S whilst preserving the Bloch law. More generally, one may ask what effect, if any, has the softening of exchange on other layer structures such as magnetic overlayers, interfaces and superlattices. We address all these questions by solving the overlayer problem first and then showing that any other layer structure can be reduced to an overlayer problem.

1. Magnetic overlayer

Consider an overlayer of N atomic planes above the (100) surface of a simple cubic ferromagnet. It is sufficient to describe this system by an exchange Hamiltonian with nearest-neighbour exchange J_{nm} between spins S_n, S_m since all the interesting physics is already contained in this model [7]. The exchange and local spin in the overlayer are arbitrary but $J_{nn+1} = J$ and $S_n = S$ in the substrate.

The surface spin deviation $\Delta M_S(T)$ is given by

$$\Delta M_S = \int_0^\infty 2\mu_B N_S(E) \left(\exp(E/kT) - 1\right)^{-1} dE, \qquad (2)$$

where $N_S(E)$ is the surface density (DOS) of spin-wave states. $N_S(E)$ is given in terms of the spin-wave Green function $G = (E - H)^{-1}$ in the mixed representation $G_{nm}(q, E)$

$$N_S(E) = (1/\pi)\ \mathrm{Tr}\ \mathrm{Im}\ G_{NN}(q, E) \qquad (3)$$

where n, m label atomic planes parallel to the surface and the trace is over the components of the wave vector q in the overlayer surface plane located at $n = N$.

To calculate G_{nm}, we have developed a new recursion method [7, 8]. The calculation of G_{nm} proceeds in the following steps:

i) the overlayer is removed from substrate;

ii) the exact $G_{00}(q, E)$ in the now exposed surface plane of the substrate ($n = 0$) is known from the classical spin-wave theory [2];

iii) the first atomic plane of the overlayer is reinstated and the matrix element G_{11} of the Green function in the new surface plane is determined recursively in terms of the old surface element G_{00};

iv) the procedure of depositing "adlayers" is repeated until the whole overlayer is "rebuilt" . After N recursion steps, we end up with the exact surface G_{NN} in terms of G_{00}.

The general recursion step from a layer n to the next layer $n + 1$ is deduced from the Dyson equation $G = G^0 + G^0 W G$, where W is a 2×2 perturbation matrix due to deposition of the adlayer $n + 1$. It takes the form

$$(G_{n+1n+1})^{-1} = \\ = \omega + W_{n+1n+1} - W_{nn+1}^2 G_{nn} / (1 - W_{nn} G_{nn}), \qquad (4)$$

where $\omega = E - 6SJ - 2SJ(\cos(q_x a) + \cos(q_y a))$ and W is expressed in terms of the local spin S_n, S_{n+1} and local exchange integrals J_{nn}, J_{nn+1}, J_{n+1n+1} within and between the layers n, $n + 1$ (see [7, 8]).

The recursion method gives an exact analytic result for the *initial* $N_S(E)$:

$$N_S(E) = (S_N/S_{N-1}) \ldots (S_1/S)\, 2N_B(E) + O\left(E^{3/2}\right), \qquad (5)$$

where $N_B(E)$ is the bulk DOS. Since $\Delta M_S(T)$ in equation (1) is normalised to $M_S(0)$, the surface spin S_N in equation (5) is cancelled and we recover the classical result $B_S = 2B_B$. It follows that neither softening of exchange nor a change of the magnetisation in an arbitrary (finite) number of at. planes near the surface has any effect on the *initial* $T^{3/2}$ law. This quite general result seems to contradict the experiment [3-6].

An explanation of this paradox is that the exact result (5) holds only for infinitesimally low spin-wave energies. Softening of the exchange perpendicular to the surface results in a rapid crossover to a new dependence $N_S(E)$. This is illustrated in figure 1 for an overlayer of N atomic planes ($N = 1, 2, ..., 30$) with a weaker exchange $J' = 0.3\ J$ between the planes. The new $N_S(E)$ leads to a second extended region of "pseudo $T^{3/2}$" law with B_S which depends strongly on J'. This is shown in figure 2 for a monolayer with $J'/J = 0.1$, 0.3 and 0.6. The curve $J'/J = 0.3$ is a perfect fit to the SPLEED data of [3] (circles). Most recent measurements [6] show that B_S / B_B varies with doping of the surface between 2 and 5.4 thus confirming that $M_S(T)$ obeys the "pseudo" rather than classical $T^{3/2}$ law. We shall now show that the "pseudo $T^{3/2}$" law is a general feature of any layer structure.

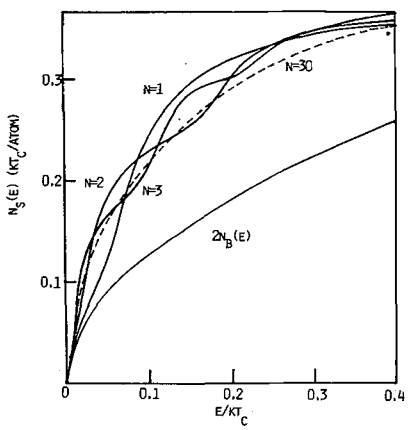

Fig. 1. – Surface DOS for an overlayer with $J'/J = 0.3$ and $N = 1, 2, ..., 30$.

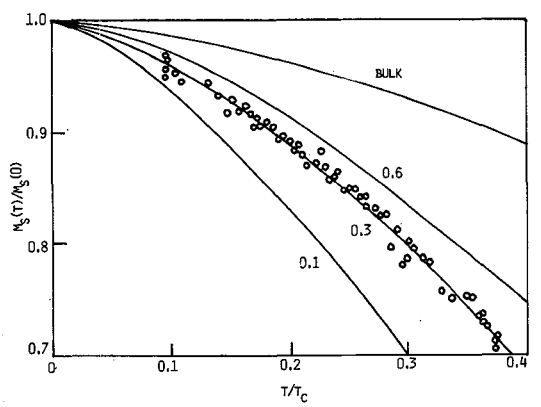

Fig. 2. – $M_S(T)$ for a surface with softened surface-bulk exchange J'/J.

2. Magnetic interfaces and superlattices

Consider an interface of N at. planes separating two homogeneous ferromagnets. To determine the local Green function G_{nn}, we pass a cleavage plane between the planes n, $n+1$ separating the interface into two independent halves. Since each half is an overlayer. The Green functions for the left G^L_{nn} and right G^R_{n+1n+1} surfaces can be calculated by the method of Sec. 1. Finally, the two halves are reconnected using the Dyson equation. It is clear from this construction that any interface is equivalent to two overlayers connected by an exchange link. The local magnetisation must, therefore, obey the "quasi $T^{3/2}$" law.

Consider next a superlattice with N at. planes in its unit cell. The superlattice is first cut by a cleavage plane into two semi-infinite halves. Given the two surface Green functions G^L, G^R, we reconnect the two halves to obtain the exact local G. It remains to calculate G^L, G^R.

Assume that the surface is at $n = 0$. We deposit on the surface, one by one, all the at. planes from the unit cell. This forms an overlayer and we use the method of Sec. 1 to express G_{NN} in its surface in terms of G_{00}. Since the surface at $n = N$ is equivalent to the old surface $n = 0$, we use the self-consistency condition $G_{NN}(G_{00}) = G_{00}$ and the recursion method for overlayers to compute G_{00} (i.e. G^L and G^R). The superlattice is reduced again to an overlayer problem.

In conclusion, we have proved that the classical result for surfaces $B_S = 2B_B$ breaks down at temperatures as low as 1 % T_C. Above these temperatures, the local $M(T)$ in any layer structure obeys the "pseudo $T^{3/2}$" law with a prefactor B_S which is determined by the local exchange. This explains not only all the existing measurements of $M_S(T)$ but offers unique opportuinity to determine the local exchange from the measured $M_S(T)$ (see [6]).

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