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On quasi twodimensional XY magnetism and superconductivity of the second kind

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Résumé. — Le rôle des fluctuations interplans associées à des boucles de vortex parallèles aux plans est considéré dans les deux problèmes couplés du magnétisme XY et de la supraconductivité de 2e espèce, en situation quasibidimensionnelle. A l’aide d’un critère simplifié, il est proposé que, pour des couplages interplans faibles, la température critique 3d est reliée à la multiplication de telles boucles ; elle est inférieure à la température de Kosterlitz et Thouless, où des boucles « normales » perçant les plans, se multiplient dans des plans indépendants.

Abstract. — The role of interplanar fluctuations associated with « parallel » vortex loops is considered in the two coupled problems of XY magnetism and superconductivity of the second kind, in a quasi-twodimensional situation. Using an admittedly simplified criterion, it is argued that, for weak interplanar couplings, the critical 3d temperature is related to the multiplication of such loops ; it should be below the Kosterlitz and Thouless temperature where « normal » vortex loops, piercing the planes, would multiply in independent planes.

Introduction.

High temperature oxide superconductors exhibit quasi-twodimensional structures, where CuO$_2$ planes with strong internal magnetic or conductive couplings, are set parallel to each other, in groups of 1, 2 or 3 planes [1-4]. The couplings between these groups are weak, while those between the planes of a group are probably more notable [5-7].

It was stressed earlier that this quasi-twodimensional arrangement was relatively favourable to high 3d magnetic or superconductive critical temperatures $T_c$, because the twodimensional fluctuations do not lower much $T_c$ from mean field values [8-10] ; this is contrary to the case of quasi-onedimensional structures met e.g. in some organic superconductors [11, 12]. Moreover, in at least some models of superconductivity, notably those with weak couplings, the quasi-twodimensional geometry can lead to especially high mean field temperatures, if the Fermi level falls near a 2d Van Hove singularity of the density of states [13, 14].

In this light, it is interesting to try and state more precisely how 2d fluctuations lower the critical temperature from the mean field value. This is wellknown for Ising or Heisenberg magnets in the geometries considered [15]. It might not be so clear for the perhaps more relevant XY magnets or for the related superconductivity case. Indeed, the purely 2d case being a borderline case [16, 17], one can expect even weak interplanar couplings to lead to large changes in behaviour.

In this paper, we shall limit ourselves to the simplest geometry of weakly coupled parallel planes, each with a square atomic lattice of parameter $a$. In the magnetic case, each atom $i$ is assumed to have a classical spin $S_i$. This is coupled to its four neighbours in the plane by an exchange interaction $J_1$, and to its two neighbours in the neighbouring planes by a weaker exchange interaction $J_2$. The distances with all neighbours will be assumed to be equal. Extensions from this simple cubic lattice to other simple and alternant structures would be straightforward and does not bring any new physics. Similar simple assumptions, to be discussed, will be made for superconductivity.
1. XT magnetism.

1.1 2d CASE. RECALL OF THE KOSTERLITZ AND THOULESS TEMPERATURE \[16, 17\]. — For an isolated plane, the magnetic energy reads

\[ \varepsilon = \frac{1}{2} J_i \sum_{i,j \text{ near } i} S_i S_j. \]  

The physics of the ferromagnetic case \((J_1 < 0)\) and antiferromagnetic case \((J_1 > 0)\) are equivalent, with a reversal of sign of \(S_i\) for one of the two sublattices. We shall consider the simpler ferromagnetic case.

The mean field critical temperature is given by \[18\]

\[ k_B T_{MF} = 4 |J_1| S^2. \]  

Owing to 2d fluctuations, the critical temperature for the average magnetisation vanishes. But the magnetic rigidity \(\langle \text{ helicity } \rangle\) \[19\] only vanishes above the Kosterlitz and Thouless temperature, given approximately by \[20\]

\[ k_B T_KT \approx 1.8 |J_1| S^2 \]  

thus of the order of the mean field value. Below \(T_KT\), the magnetic susceptibility and magnetic coherence length are infinite.

\(T_KT\) is the temperature above which "normal" vortex lines, piercing the XY planes (i.e. magnetic critical points) multiply spontaneously. It can be approximately estimated by an argument first developed for 3d melting \[21, 22\]. Thus a pair of vortex lines, of opposite strengths \(\pm 2\pi\), at a distance \(d\) from each other, in an otherwise perfect magnetic arrangement, have an internal energy \[23\]

\[ U = 2 \pi |J_1| S^2 \ln \left(\frac{d}{a}\right). \]  

This is derived from the fact that, to a spatial variation of the angle \(\phi\) of the axis \(S\), one can relate an elastic (or spin wave) energy density

\[ \frac{1}{2} K_1 a^2 (\text{grad } \phi)^2 \]  

where the elastic constant \(K_1\) is related to \(J_1\) by

\[ K_1 = J_1 S^2 / a^3 \]  

if the "thickness" of the plane is assumed to equal the lattice parameter \(a\) in the plane. The line tension of a vortex is given classically by summing this energy from \(a\) to \(R\):

\[ \tau(R) \approx \pi K_1 a^2 \ln \left(\frac{R}{a}\right). \]  

The equilibrium concentration at temperature \(T\), when small, is given by

\[ C_T \equiv \exp \left(\frac{-U}{k_B T}\right). \]  

The interactions between vortex pairs begin to shield the mutual interaction in a pair when

\[ C_T \approx (a/d)^2. \]  

Hence \[24\]

\[ k_B T_KT \approx U / 2 \ln (d/a) \approx \pi |J_1| S^2, \]  

independent of \(d\) and near enough to \(3\).

1.2 THE QUASI-TWO-DIMENSIONAL CASE. — An interplanar coupling energy

\[ \varepsilon' = \frac{1}{2} J_{\perp} \sum_{i,z} S_i S_z \]  

is added between pairs of opposite sites \(i, l\) on neighbouring planes. Again the ferromagnetic case \((J_1 < 0)\) is considered.

It is then usually argued \[15\] that, below \(T_KT\), the infinite susceptibility will give, for any strength of the interplanar coupling \(J_{\perp}\), a 3d coupling between planes. Above \(T_KT\), the coherence length for an isolated plane varies as

\[ \xi(T) \approx a \exp \left(\frac{\pi}{2} \left(\frac{T}{T_KT} - 1\right)^{-1/2}\right). \]  

Within mean field, one can expect 3d ordering up to a temperature \(T_c\) such that thermal energy equals the interplanar coupling over an area of size the coherence length:

\[ k_B T_c \approx |J_{\perp}| S^2 \xi^2(T_c)/a^2. \]  

Hence, with \(3\) or \(10\),

\[ k_B T_c \approx k_B T_KT[1 + \pi^2/4 \ln^2(\xi/a)] \approx k_B T_KT[1 + \pi^2/2 \ln^2|J_1/J_{\perp}|]. \]  

This is larger than \(T_KT\).

This type of reasoning is inspired by similar reasonings for quasionedimensional cases or for the quasitwodimensional Heisenberg one. Two objections can be raised:

— The 2d XT magnetic case being a borderline case, any small perturbation such as the interplanar coupling \(J_{\perp}\) can produce a large effect. Indeed, in this case, \(T_c\) is assumed to raise from 0 to above \(T_KT\) for any \(J_{\perp} \neq 0\) ; but there is no obvious reason why \(T_KT\) should still be meaningful for \(J_{\perp} \neq 0\) ;

— more technically, the argument about threedimensional \(T_c\) being necessarily larger than \(T_KT\) because of infinite susceptibility relies on an analysis
of the 2d fluctuations below $T_{KT}$ in terms of long wavelength and weak amplitude spin waves. Below $T_{KT}$ but near enough to it, the interplanar fluctuations can however lead to the production of parallel (interplanar) vortex loops. The characteristic temperature for 3d ordering should then be their temperature of spontaneous multiplication, if this is below $T_{KT}$.

We shall use a simplified model analogous to that leading to equation (10), and shall therefore compare the temperature of multiplication obtained in this way to that estimate of $T_{KT}$.

More precisely, we can consider two types of vortex loops: perfect or imperfect.

Perfect parallel vortex loops are loops of rotation $2\pi$ with their core lying between two neighbouring planes. Their line tension can be written as

$$\tau(R) = \pi \sqrt{|J_1 J_\perp|} \frac{S^2}{a} \ln \frac{eR}{2\eta}$$

with

$$\eta/a = \sqrt{|J_1/J_\perp|},$$

a standard result for a vortex line with a split core of width $\eta$ along the $xy$ plane (25, 26), as first analysed by Peierls [27] (cf. appendix B).

Writing the internal energy of such a loop as

$$U \equiv \pi d \tau(d),$$

the temperature of spontaneous multiplication is then given by (8, 9):

$$k_B T_A \approx \frac{\pi^2 d}{2a} \sqrt{|J_1 J_\perp|} \frac{S^2}{a} \times$$

$$\times \ln \left[ \frac{ed}{2a} \sqrt{|J_\perp/J_1|} \right] / \ln \left( \frac{d}{a} \right).$$

$T_A$ increases with $d$. Its minimum value is obtained for the minimum value of $d$ which is physically significant. Because of the core splitting of the vortex, we have

$$d \geq \eta.$$  

(19)

(18) then leads to

$$k_B T_A^{\text{min}} \approx (1 - \ln 2) \pi^2 |J_1| S^2 \ln |J_1/J_\perp|.$$  

(20)

Imperfect vortex loops, of rotation less than $2\pi$, would surround an area of misfit due to the $J_\perp$ coupling. Two characteristic cases are as follows.

Rotation $\pi$:

$$U \equiv \frac{\pi^2 d}{4} \sqrt{|J_1 J_\perp|} \frac{S^2}{a} \ln \frac{ed}{2\eta} + \frac{\eta d^2}{2a^2} 2|J_\perp| S^2.$$  

(21)

The minimum temperature of multiplication, for $d \equiv \eta$, is

$$k_B T_B^{\text{min}} \approx \pi |J_1| S^2 \left[ \frac{\pi}{4} (1 - \ln 2) \right] / \ln |J_1/J_\perp|.$$  

(22)

Rotation $\pi/2$:

$$U \equiv \frac{\pi^2 d}{16} \sqrt{|J_1 J_\perp|} \frac{S^2}{a} \ln \frac{ed}{2\eta} + \frac{\eta d^2}{a^2} |J_\perp| S^2.$$  

(23)

With $(1 - \ln 2) \pi \approx 1$, we see that these three temperatures are nearly equal. From (2) and (10), we can write

$$k_B T_A^{\text{min}} \approx k_B T_B^{\text{min}} \approx K_B T_c^{\text{min}} \approx k_B T_{MF}$$  

$$\approx \frac{k_B T_{KT}}{\ln |J_1/J_\perp|} \approx \frac{k_B T_{MF}}{\ln |J_1/J_\perp|}.$$  

(24)

According to this admittedly rough reasoning, this is the temperature at which the coherency between planes is lost and 3d order destroyed. This temperature tends to zero with $J_\perp$, which is physically more reasonable. Furthermore the distortions produced above this temperature, owing to the multiplication of parallel vortex loops, probably destroy the helicity characteristic of 2d long range order below $T_{KT}$ in independent planes [34]. Thus, at least for strong enough values of $J_\perp$, the Kosterlitz and Thouless temperature $T_{KT}$ might lose any physical significance, only a 2d short range order persisting above $T_A \approx T_B \approx T_c$.

2. Superconductivity of the second kind.

2.1 RECALL OF THE 2d CASE. — An analysis similar to that of the $XY$ magnetic one can be made [28]. There are however some differences.

From London’s equation where $\lambda_1$ is the penetration depth within a plane,

$$\lambda_1^2 \Delta H = H,$$  

(25)

one finds that the field in a vortex line behaves at long range ($r > \xi_1$) as

$$H \approx \frac{\Phi_0}{2\pi r} \exp \left( - \frac{r}{\lambda_1} \right)$$  

(26)

where

$$\Phi_0 = \frac{2\pi \hbar c}{2e}$$  

(27)

is the flux quantum. Adding a core energy due to the destruction of superconductivity for $r < \xi_1$, the coherence length, one can write approximately for
the line tension of a « thermal » vortex (singular point)

\[ \tau = \frac{\Phi_0^2}{16 \pi^2 \lambda_1^2} \ln \frac{\lambda_1}{2 \xi_1} + \frac{\pi \xi_1^2}{a^3} k_B T_1 \]  

(28)

where \( T_1 \) is the mean field superconductivity temperature within the plane.

The energy of a pair of such vortices of opposite signs, at a distance \( d < \lambda \), is then

\[ U = \frac{\Phi_0^2 a}{8 \pi^2 \lambda_1^2} \ln \frac{d}{2 \xi_1} + \frac{2 \pi \xi_1^2}{a^3} k_B T_1 \]  

(29)

The Kosterlitz and Thouless temperature is then given by

\[ k_B T_{KT} = U/2 \ln \left( d/a \right). \]  

(30)

Rough estimates give, for a classical BCS coupling [29],

\[ \lambda_1 \approx \left( \frac{m_1 c^2}{2 \pi n_s \hbar^2} \right)^{1/2} \]  

(31)

\[ \xi_1 \approx 2 \hbar v_1 / \pi \Delta \]  

(32)

with

\[ 2 k_B T_1 \approx 3.5 \Delta \]  

(33)

where \( n_s \) is the number of electrons per unit volume, of order \( (a^3)^{-1} \) in \( \text{CuO}_2 \) planes. The ratio of \( \Phi_0^2 c/8 \pi^2 \lambda_1^2 \) to \( 2 \pi (\xi_1^2/a^2) k_B T_1 \) in (29) is then of the order of the ratio of \( \Delta \) to \( 1/2 m^* v_1^2 \), thus very small compared with unity. As a result, \( k_B T_{KT} \) decreases with increasing \( d \) for any reasonable value of \( \xi_1/a \). The minimum value is, for \( d \approx \lambda \),

\[ k_B T_{KT}^{\text{min}} \approx \Phi_0^2 a / 16 \pi^2 \lambda_1^2. \]  

(34)

Using (31), one can also write

\[ k_B T_{KT}^{\text{min}} \approx \frac{\pi h^2 n_s a}{4 m_1} \approx \frac{\pi h^2}{4 m_1 \hbar^2} \approx \frac{k_B a}{12 \pi} E_M \]  

(35)

where \( E_M = h^2 k_M^2/2 m \) is the Fermi energy.

We see that the two cutoffs \( \xi_1 \) and \( \lambda_1 \), equation (28), do not play any significant role in the definition of \( T_{KT} \). But because the main contribution to the line tension of a vortex is long range, \( T_{KT} \) essentially depends on \( \lambda_1 \), and not on the energy of the superconductive state. Furthermore the estimate (35) shows that it is definitely above the mean field critical temperature.

This means that \( T_{KT} \) has little chance of having a physical meaning, even for isolated planes.

Formulae have been given for the case of « pure » superconductors where the mean scattering length \( l \) is larger than \( \xi_1 \). In the opposite case [30], \( \tau \) and \( U \), and thus \( T_{KT} \), are reduced in the ratio \( l/\xi_1 \). This is a somewhat unlikely limit for oxide superconductors, where \( \xi_1 \approx 20 \) to 30 Å.

2.2 QUASI TWO DIMENSIONAL SUPERCONDUCTIVITY. — We shall only consider here classical BCS coupling, where there are two limits of weak interplanar coupling: the anisotropic limit and the Josephson junction limit. It is however likely that similar considerations would apply whatever the microscopic origin of superconductive coupling.

In the anisotropic limit, electrons move coherently from plane to plane, with an effective mass \( m_\perp \) (or an effective transfer integral \( t_\perp \)). \( m_\perp \) is much larger than the effective mass \( m \), within the planes (or \( \eta \gg t_\perp \)).

From (31, 33) one deduces that the values of \( \lambda_\perp / \xi_\perp \approx (m_\perp / m_1)^{1/2} \approx (\eta / t_\perp)^{1/2} = \alpha \).  

(36)

For a vortex line « parallel » to the \( xy \) plane along the \( y \) axis, equation (25) is now replaced by

\[ \lambda_\perp \frac{\partial^2 H}{\partial x^2} + \lambda_\perp \frac{\partial^2 H}{\partial z^2} = H. \]  

(37)

The use of reduced coordinates

\[ x' = x, \quad z' = z \sqrt{\lambda_1 / \lambda_\perp} = \alpha^{-1/2} z \]  

(38)

leads to the solution

\[ H = \frac{\Phi_0'}{2 \pi r'} \exp \left( - \frac{r'}{\lambda_\perp} \right) \]  

(39)

with

\[ \Phi_0' = \alpha^{-1/2} \Phi_0. \]  

(40)

Hence, for a loop of diameter \( d \), an energy

\[ U = \frac{\pi d}{a} \left[ \frac{\Phi_0^2 a}{16 \pi^2 \lambda_1 \lambda_\perp} \ln \frac{ed}{2 \xi_1} + \frac{\xi_1 \xi_\perp}{a^2} k_B T_\perp \right] \]  

(41)

and a temperature of spontaneous multiplication

\[ k_B T_A \approx U/2 \ln \left( d/a \right) \]  

(42)

\( T_\perp \) is the mean field superconductive interplanar coupling.

As for the \( XY \) model, the minimum temperature of spontaneous multiplication should be obtained for the loop of minimum diameter of physical significance:

\[ d \approx \xi_1. \]  

(43)

For large values of \( \alpha \), one expects

\[ \xi_\perp = a. \]  

(44)
as seems indeed observed in superconductive oxides. Hence
\[ k_B T_A^{\text{min}} = \frac{\pi \alpha}{2} \left[ \frac{\Phi_0^2 a}{16 \pi^2 \lambda_f^2} (1 - \ln 2) + \alpha k_B T_\perp \right] / \ln \alpha. \] (45)

With the rough assumption
\[ T_1 / T_\perp = \alpha^2, \] (46)
the same reasoning as for (29) shows that, in (45), the second term is much larger than the first one. Hence
\[ k_B T_A^{\text{min}} = \frac{\pi \alpha^2 k_B T_\perp}{2 \ln \alpha} = \frac{k_B T_1}{\ln \alpha}. \] (47)

One can also imagine imperfect parallel vortex loops, as for the XY model. It is easy to check that, with the same assumptions, they lead to similar results for the temperature of spontaneous multiplication.

For large values of \( \alpha \), it is probably more reasonable to consider the Josephson junction limit [31]. The interplanar coupling temperature \( T_\perp \) is then related to the intraplanar one by a relation such as [8]
\[ T_1 / T_\perp = (k_B T_1 / T_\perp)^2 = \alpha^2. \] (48)

One can then define, in each plane, a phase of the superconductive order parameter with variations within each plane and from plane to plane related to \( T_1 \) and \( T_\perp \) respectively. The analysis of the non superconductive core is similar to that in the magnetic case. For a « parallel » vortex line, its dimensions parallel and normal to the xy plane will be given by
\[ \frac{1}{\alpha^2} \eta = r_\perp = \eta \cdot \alpha. \] (49)

Equation (41) still applies, with \( \xi \) replaced by \( r \). Hence again, with the first term still negligible,
\[ k_B T_A^{\text{min}} = k_B T_1 / \ln \left| T_1 / T_\perp \right| \] (50)
an expression used previously without justification by the author [8, 9].

Discussion.

The general conclusion of this paper is that, in the quasi twodimensional geometry, the 3d order parameter should vanish above a critical temperature which is of the order of the mean field 2d critical temperature divided by the logarithm of the ratio of intra and interplanar couplings. This formula is the same as that valid in the Heisenberg case. This temperature, which tends to zero for vanishing interplanar coupling, is always below the 2d Kosterlitz and Thouless temperature. It is suggested that this last temperature loses its physical significance, at least for sizeable interplanar couplings, but that 2d fluctuations should be observed up to the mean field 2d temperature.

In trying to apply these results to oxide superconductors, care must be taken of the following complications.

In the magnetic phases, the spin orbit coupling is large enough for an XY model to be more relevant than a Heisenberg one [9]. However it is not yet clear whether a classical model is relevant for atomic moments which are of the order of one Bohr magneton or less. Quantum fluctuations should certainly be taken into account if the corresponding electrons are localised; and one knows indeed that, for localised \( S = 1/2 \) spins, the Kosterlitz and Thouless temperature (3) is replaced by [32]
\[ k_B T_{KT} = 0.7 S (S + 1). \]

For delocalised electrons, this is probably not the case; the validity of (1, 11) is otherwise approximative. Furthermore, in \( La_{2-x} Sr_x Cu O_4 \), \( J_\perp \) comes from a rotation of the oxygens around each Cu which arises in the orthorhombic phase. The corresponding Dzyaloshinskii Moriya term induces the moments to rotate out of the xy planes, in a definite crystallographic direction. The situation might therefore be similar to an Ising model more than to an XY one. In \( Y Ba_2 Cu_3 O_6 \), the magnetic planes are grouped in close pairs. The geometry is then slightly different from that considered here.

In the superconductive phases, it is not clear whether BCS applies, and whether one is in the Josephson junction case. Also, for \( Y Ba_2 Cu_3 O_7 \) as for the newer Bi or Tl base compounds, the conductive planes are grouped in two or three (or more), thus altering somewhat the simple geometrical arrangement considered here.

In all these cases, the same arguments should apply qualitatively to predict 3d order parameters which increase continuously from zero with the strength of interplanar coupling in a logarithmic way as in the Heisenberg case [33]. This temperature should be below the mean field 2d temperature, up to which one can expect 2d fluctuations to be observed. The Kosterlitz and Thouless 2d temperature should probably lose any physical significance at least for strong enough couplings. In the cases of regrouping of the planes in two’s or three’s or \( n \), one should expect the meanfield 2d temperature to be independent of regrouping as long as the interplanar couplings within each group is not too large. However, if it is significantly larger than the intergroup
couplings, they could reduce the importance of 2d fluctuations and increase the 3d critical temperatures. This point will be studied in another paper.

These predictions could be usefully checked by computer studies on crystals of finite sizes.

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Appendix A.

Peach and Koehler force.

From a total elastic energy
\[ \varepsilon = \frac{1}{2} Ka^2 \int (\text{grad } \phi)^2 \, d\tau, \]
one deduces, by a variation of \( \phi \), the equilibrium condition
\[ \Delta \phi = 0. \]

Let \( \phi_1 \) and \( \phi_2 \) be two possible equilibrium solutions. Then \( \phi_1 + \phi_2 \) is also one. Its energy is
\[ \varepsilon = \varepsilon_1 + \varepsilon_2 + \varepsilon_{12} \]
where
\[ \varepsilon_{12} = Ka^2 \int \gamma \phi_1 \cdot \text{grad } \phi_2 \, d\tau \]
\[ = Ka^2 \left\{ \int \phi_1 \Delta \phi_2 \, d\tau - \int \phi_2 \text{grad } \phi_1 \cdot dS \right\}. \]

At equilibrium, the first term vanishes, except along the core of a singularity of \( \phi_2 \). The second term vanishes far from any vortex line. However, if \( \phi_2 \) is due to a vortex line \( L_1 \), \( S \) must contain a « Volterra cut » bordering \( L_2 \). Over the two lips \( S_2, S_2^* \) of the cut, \( \phi_2 \) varies by \( 2n_2 \pi \). Hence
\[ \varepsilon_{12} = 2n_2 \pi Ka^2 \int \text{grad } \phi_1 \cdot dS. \]

This gives the energy of interaction of the vortex line \( L_2(2n_2 \pi) \) with an « external » distortion \( \phi_1 \).

Writing
\[ dS = dx \wedge dl \]
where \( dl \) is along \( L_2 \) and \( dx \) the direction normal to it along \( S_2 \),
\[ \varepsilon_{12} = 2n_2 \pi Ka^2 \int \text{grad } \phi_1 (dx \wedge dl) = \int_{S_2} \mathbf{F} \, dl \, dx \]
where
\[ \mathbf{F} = 2n_2 \pi Ka^2 (\text{grad } \phi) \wedge \frac{dl}{dl} \]
is the Peach and Koehler force associated with \( \phi_1 \).

For two parallel vortex lines of opposite strengths \( \pm 2 \pi \) at distance \( d \) from each other,
\[ \varepsilon_{12} = 2 Ka^2 \ln (R/d). \]

Hence equation (7).

Appendix B.

Peierls splitting of a parallel vortex line in the quasi twodimensional XY magnetic case.

We consider the magnetic lattice of the text, where each site \( i \), with classical spin \( S_i \) in the \( xy \) plane, has four neighbours \( j \) in the same plane and one neighbour \( l \) in each neighbouring parallel plane. The magnetic energy is written as
\[ \varepsilon = \frac{1}{2} \sum_{i,j \text{ near to } i} J_{ij} S_i S_j + \frac{1}{2} \sum_{i,l \text{ near to } i} J_{il} S_i S_l. \]

We treat the ferromagnetic case \( (J_1 \text{ and } J_{ll} < 0) \). Antiferromagnetic cases \( (J_1 \text{ or } J_{ll} > 0) \) follow with suitable reversals of one spin direction over two.

We consider a parallel vortex line of rotation \( 2 \pi \), which sits parallel to the \( y \) axis, between two successive \( xy \) planes. On each site \( i \), the direction of \( S_i \) is measured by its angle \( \phi \) with the \( x \) axis in the \( xy \) plane.

In (B.1), the Peierls approximation consists in treating explicitly the interactions, \( i, l \) between the two \( xy \) planes on either sides of the vortex line, while all other interactions are treated in the elastic limit.

The splitting of the vortex line along the \( x \) direction is represented by a change \( \delta \phi = \phi^+ - \phi^- \) of the orientations of \( S \) on the \( xy \) planes just above and below the vortex line. \( \delta \phi \) increases with \( x \) from 0 to \( 2 \pi \); the vortex line \( 2 \pi \) is replaced by a continuous distribution of infinitesimal vortex lines of strength \( d\delta \phi/dx \) for each slice \( dx \) along the \( xy \) plane.

The total line tension reads, in this approximation,
\[ \tau = K_\perp a^2 \sum_i \cos (\delta \phi_i - 1) + \frac{1}{2} \sqrt{K_\perp K_1} \times \int_{-R}^R \int_{-R}^R \frac{d \delta \phi(x') \delta \phi(x)}{x' - x} \, dx \, dx'. \]
where, as in the text,

\[ K_1 = \frac{J_1 S^2}{a} \quad \text{and} \quad K_\perp = \frac{J_\perp S^2}{a^3}. \quad (B.3) \]

The first term is the short range « stacking fault » energy due to the vortex, expressed per unit length along the y axis.

The second term is the long range elastic energy. It is most easily obtained using reduced coordinates

\[ x' = x, \quad z' = \frac{a}{c} \sqrt{\frac{K_1}{K_\perp}} z, \quad (B.4) \]

for which the elastic constant is isotropic and equal to \( K_1 \). The second term is then half the work done to produce a Volterra cut along \( x_y \), with a local relative rotation \( \delta \phi(x) \), under the resolved « stress » \( K_1 a^2 \text{grad} \phi(x) \) due to the vortex. In isotropic conditions,

\[ \Delta' \phi = 0 \quad (B.5) \]

and the rotation \( \phi \) along the \( xy \) plane is given by adding the contributions of the various parts of the vortex. Hence

\[ K_1 a^2 \text{grad} \phi(x) \, dS = \sqrt{K_\perp} K_1 a^2 \int_{-R}^{R} \frac{d \delta \phi(x')}{dx'} \, dx'. \quad (B.6) \]

Equation (B.2) follows.

In the limit \( K_1 \gg K_\perp \) considered in the text, the second term in (B.2) dominates. One can then replace in the first term the summation over \( i \) by an integration over \( x \). The condition of equilibrium

\[ d\tau/d\delta \phi = 0 \quad (B.7) \]

leads then, with an integration by parts, to the condition of local equilibrium

\[ K_\perp a \sin \delta \phi = \sqrt{K_\perp} K_1 a^2 \int_{-R}^{R} \frac{d \delta \phi(x')}{dx'} \, dx'. \quad (B.8) \]

The corresponding soliton solution reads

\[ \delta \phi = \pi + 2 \arctg \frac{x - \alpha}{\eta} \quad (B.9) \]

where

\[ \eta = \sqrt{\frac{K_1}{K_\perp}} a. \quad (B.10) \]

Injecting (B.9, B.10) into the formula for the line tension gives, if only the leading terms in \( K_1/K_\perp \) are kept, to

\[ \tau = \pi \sqrt{K_\perp K_1 a c \ln \frac{eR}{2\eta}}. \quad (B.11) \]

References

[6] Hybertsen, M. S. and Mattheiss, L. F., 1988 (to be published);
Massida, S., Yu, J. and Freeman, A. J., 1988 (to be published);