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On quasi twodimensional order in XY magnets or superconductors of the second kind.
Influence of multiple layering

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Résumé. — Un raisonnement concernant la multiplication spontanée de boucles de vortex interplanaires est étendu aux structures à couches multiples. Il est suggéré qu'un couplage plus fort entre plans magnétiques à l'intérieur d'un groupe que de groupe à groupe décroît fortement les fluctuations bidimensionnelles. Cet effet devrait augmenter la température critique tridimensionnelle à peu près en proportion du nombre de plans dans chaque groupe, si les autres paramètres restent constants. Cet effet peut aussi jouer un rôle important dans le cas de la supraconductivité. La situation des oxydes supraconducteurs est discutée de ce point de vue.

Abstract. — Extending an earlier reasoning about spontaneous multiplication of interplanar vortex loops, it is suggested that multiple layering of magnetic planes, more strongly coupled within each group than from group to group, decreases strongly the two dimensional fluctuations. This should increase the three dimensional critical temperature roughly proportionately to the number of planes within each group, if other parameters remain equal. It is argued that this effect could also play an important role in the superconducting case. The situation of oxide superconductors is discussed in this light.

Introduction.
It has been recently suggested [1] that, in a simple quasi twodimensional XY magnetic case, the threedimensional critical temperature $T_c$ is dominated by the spontaneous multiplication of interplanar vortex loops, and not by the Kosterlitz and Thouless one [2] of vortex loops piercing the magnetic planes. Using a simple cubic model, where $J_1$ is the exchange interaction between planes and $J_{\perp}$ that from plane to plane, one obtains

$$k_B T_c \approx 3 |J_1| S^2/\ln |J_1/J_{\perp}|.$$  \hspace{1cm} (1)

For $|J_1/J_{\perp}| \gg 1$, $T_c$ is then definitely smaller than the mean field [3] temperature $T_{MF}$ or the Kosterlitz and Thouless one $T_{KT}$, which are of order

$$k_B T_{MF} \approx k_B T_{KT} \approx |J_1| S^2$$ \hspace{1cm} (2)

where $2 < \alpha < 4$.

Similar results apply to quasi twodimensional superconductors of the second kind, at least in the Josephson junction coupling limit [4]. $|J_1| S^2$ and $|J_{\perp}| S^2$ are then replaced by the corresponding meanfield intra and interplanar superconductive couplings.

The purpose of this note is to extend these results to multiply layered structures with a view to the new oxide superconductors [5-7]. For simplicity sake, we still assume the magnetic or conductive atoms to be on a simple cubic lattice of parameter $a$, with nearest neighbours interactions. But, in the $XY$ magnetic case, we assume now that the $xy$ planes are regrouped in families of $n$ neighbouring planes with interactions $J_{\perp}$, while the interactions between planes of different groups are $J_{\perp}$. It is assumed that

$$|J_{\perp} | \ll |J_{\perp}| \ll |J_1|.$$ \hspace{1cm} (3)

As in the previous discussion, we limit ourselves to ferromagnetic interactions. Extensions to simple antiferromagnetic cases or to topologically equivalent lattices are straightforward and do not bring any new physics. Similar assumptions will be made for superconductors of the second kind.

Layered structures.
Looking first at the $XY$ magnetic case, it is clear that the creation of an interplanar vortex loop of diameter $d$, parallel to $xy$, will require its minimum energy if its core lies between groups of planes of the layered structure, in a region of weak coupling $|J_{\perp}|$, in preference to within a group of planes with the stronger coupling $J_{\perp}$. 

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The Peierls analysis of its energy \([8, 9]\) requires to define the average long range elastic energy associated with the gradient of the angle \(\phi\) which each spin \(S\) makes within its \(XY\) plane. It is fairly obvious that, if
\[
|J_\parallel| / |J_\perp| \gg n
\]
as assumed here, the variation of \(\phi\) with \(z\) concentrates practically between the groups of \(n\) planes, while there is no significant variation of \(\phi\) with \(z\) within each group (cf. Appendix A). Then, for the low temperature description of a vortex loop, each group of \(n\) planes can be replaced topologically by a single plane with intraplane coupling \(nJ_1\), while the coupling \(J_\perp\) remains between the groups.

The energy \(U(d)\) of interplanar vortex loops of diameter \(d\) is then given, by a standard computation using the Peierls approximation \([1,10,11]\), as
\[
U(d) \equiv \pi^2 \frac{n|J_1| J_\perp}{a} S^2 d \frac{ed}{2 r_0}
\]
where \(r_0\) is the core diameter of the vortex loop measured along the \(xy\) plane. Their equilibrium concentration is
\[
c = \exp \left( - \frac{U(d)}{k_B T} \right)
\]
and the temperature of spontaneous multiplication occurs for \([12]\)
\[
c = (a/d)^2.
\]
Hence
\[
k_B T_c(d) \approx U(d)/2 \ln \left( d/a \right).
\]

\(T_c(d)\) increases with \(d\). Its minimum value \(T_c\) corresponds to the minimum value of \(d\) of physical significance, hence for
\[
d \approx r_0.
\]
A standard computation gives here \([8]\) to \([11]\)
\[
r_0 \approx \sqrt{n|J_1| J_\perp / a}.
\]
Hence \((1)\)
\[
k_B T_c \approx \beta n |J_1| S^2 / \ln \left( n |J_1| J_\perp \right)
\]
where
\[
\beta = \pi^2 (1 - \ln 2) \approx 3 = \alpha.
\]
A similar analysis can be made for superconductors strongly of the second kind, where \(|J_1| S^2\) and \(|J_\parallel| S^2\), \(|J_\parallel| S^2\) have to be replaced by mean field superconductive couplings within and between planes. It should be especially valid in the limit of very small and anisotropic coherence lengths, as seems to be observed in superconductive oxides. A Josephson junction coupling might then be valid to describe the intergroup couplings; and one can then expect a result similar to \((5, 6)\), i.e.
\[
k_B T_c \equiv nk_B T_1 \ln \left( n T_1 / T_\perp \right).
\]

Here, \(T_1\) and \(T_\perp\) are meanfield temperatures measuring the superconductive couplings within planes and between groups.

**Variation of \(T_c\) with \(n\).**

According two \((5)\) and \((7)\), one should expect \(T_c\) to increase with \(n\). As \(|J_1|/J_\perp|\) is probably much larger than unity (typically at least 5 or 10), \(T_c\) should be roughly proportional to \(n\), at least for moderate values of \(n\) (typically \(n < 5\)) and if all other parameters remain equal.

Table I shows indeed that this seems to be roughly the case, both for the antiferromagnetic case \((T_N)\) and the superconductive one \((T_S)\).

<table>
<thead>
<tr>
<th>(n)</th>
<th>(T_c)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.1</td>
</tr>
<tr>
<td>2</td>
<td>0.2</td>
</tr>
<tr>
<td>3</td>
<td>0.3</td>
</tr>
<tr>
<td>4</td>
<td>0.4</td>
</tr>
</tbody>
</table>

Besides the question of constancy of parameters, discussed below in details, there is an intrinsic limitation of the increase of \(T_c\) with \(n\). It is that
\[
T_c \leq T_{MF}.
\]
The meanfield temperature \(T_{MF}\) is still given by \((2)\) because, with condition \((3)\), the planes fluctuate independently at these high temperatures. There should therefore be a saturation of the increase of \(T_c\) with \(n\) for
\[
n \approx n_c \equiv \ln |J_1|/J_\perp| \quad \text{or} \quad \ln |T_1|/T_\perp|,
\]
which, as we have stressed, is probably of the order of a few units \([13, 14]\), and certainly not larger than 4 to 5.

If this point of view is right, one should expect, if \(n < n_c\), strong 2d fluctuations to be observed for
\[
T_c < T < T_{MF},
\]
thus over a range which should decrease with increasing values of \(n\). One can also expect, in the superconductive case, to observe pseudogap excitations on the conductive planes that should correspond to \(T_1 > T_c\) for \(n < n_c\); the ratio \(T_1/T_c\) should decrease with increasing \(n\) in this range.

These predictions on fluctuations seem also qualitatively coherent with experiments. A detailed discussion on the question of constancy of other parameters however suggests possible deviations from these perhaps oversimple predictions.

**The magnetic cases.**

So far, only the \(La_2CuO_4\) and \(YBa_2Cu_3O_6\) families show antiferromagnetism, with respectively \(n = 1\) and 2. This is at least approximately of the \(XY\) type \([14, 15]\), and the observed \(T_N\) are in the ratio 420/240 (cf. Tab. I), thus of the right order of magnitude 2/1.
Table I. — Variations with $n$ of $T_N$ and $T_S$.

<table>
<thead>
<tr>
<th>$n$</th>
<th>$T_N$</th>
<th>$T_S$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>La$_2$CuO$_4$</td>
<td>240</td>
</tr>
<tr>
<td>2</td>
<td>YBa$_2$Cu$_3$O$_6$</td>
<td>420</td>
</tr>
<tr>
<td>3</td>
<td>YBa$_2$Cu$<em>3$O$</em>{10}$</td>
<td>120</td>
</tr>
</tbody>
</table>

There are also good indications from NMR studies [16] in the YBa$_2$Cu$_3$O$_6$ family that the neighbouring CuO$_2$ planes are coupled magnetically rather strongly through direct Cu-Cu interactions (and not through the Y atoms); this is coherent with the sizeable overlaps and transfer integrals deduced from band computations [17].

Finally the 2d magnetic fluctuations are very strong up to at least 400 K in [15] La$_2$CuO$_4$, while they might be more modest [18] in YBa$_2$Cu$_3$O$_7$. This explains why the $XY$ model is valid well above $T_N$: the spin anisotropy per Cu atom is modest, but not that per coherently fluctuating zone $\xi$ (coherence length) [14].

There are however some (probably minor) questions to be resolved in a more exact analysis. Quantum fluctuations of the spins should perhaps be taken into account. For pure 2d cases, one knows that this does not alter the Kosterlitz and Thouless temperature much [19].

In La$_2$CuO$_4$, the magnetic coupling $J_\perp$ is due to the small orthorhombic distortion, and vanishes in the tetragonal phase, contrary to YBa$_2$Cu$_3$O$_6$. It is therefore expected to be especially weak and somewhat temperature sensitive [13]. This, however, only weakly alters the logarithmic term in $T_N$. Furthermore, the spin orbit coupling induces in the $XY$ plane a magnetic anisotropy due to the orthorhombic distortion [20]; one is therefore somewhat intermediary, near $T_N$, between an Ising and an $XY$ case.

In YBa$_2$Cu$_3$O$_6$, $J_\perp$ is also expected to be small, because of an indirect coupling through the CuO chains.

The superconductive cases.

Here, compounds with $n = 1, 2, 3$ and perhaps more are known. A striking and systematic increase of $T_S$ with $n$ is observed, again roughly proportional to $n$ for these small values [33], which are reasonably expected to be below $n_c$, equation (8) (Tab. I).

Moreover a « gap » observed by NMR on the CuO$_2$ planes, more likely to be representative of $T_1$ than $T_S$, is larger than expected in a standard BCS relation to $T_S$, at least in [21] La$_{2-x}$Sr$_x$CuO$_4$ and in [16, 22] YBa$_2$Cu$_3$O$_7$. The existence of 2d superconductive fluctuations for $T_S < T < T_1$ and of a pseudogap related to $T_1$ in that range have not been clearly established, however.

This tentative interpretation relies on the assumptions that the coupling meanfield temperatures $T_1$, $T_\perp$, $T_\parallel$ are equal in all compounds and follow a condition similar to (3):

$$ T_\perp < T_\parallel < T_1. $$

As we shall see, it is reasonable to expect condition (9) to be fulfilled; but $T_1$ might well vary by a factor 2 from compound to compound. The agreement of table I with simple predictions might be due, to some degree, to a compensation of (modest) errors. We shall base this discussion on a weak coupling BCS description, although it is quite possible that other models would lead to similar conclusions.

In the weak coupling BCS description, $T_1$, $T_\perp$, and $T_\parallel$ are related to the corresponding transfer integrals $t_1$, $t_\perp$, and $t_\parallel$ between Cu atoms (or equivalently to the corresponding effective masses). Now transport [23] and optical properties [24] suggest

$$ t_\perp/t_1 \approx 10^{-2}, $$

in agreement with band computations [17, 25-27] which also give (Appendix B)

$$ t_\parallel/t_1 \approx 10^{-1}. $$

The weak ratio of $t_\perp/t_1$ suggests a Josephson coupling limit for the coupling between groups, leading very approximately to [14]

$$ T_\perp/T_1 \approx \left( \frac{t_\perp}{3.5 k_B t_1} \right)^2. $$

With [25] $t_1 \approx 0.8$ eV and $T_1 \approx 40$ K, this is indeed small compared with unity. Concerning $T_\parallel$, the ratio $T_\perp/T_1$ is probably too large for a Josephson junction model to apply between the planes of one group. It is however clear that it is both much larger than $T_\perp$ and smaller than $T_1$. Thus condition (9) is certainly fulfilled.

Concerning now the constancy of $T_1$ from compound to compound, this can be at best only approximate. It is true that, in the BCS weak coupling limit, the Cu d $x^2$, $y^2$-O p(x or y) antibonding band is always nearly half filled and near a Van Hove anomaly which leads to large values [28] to [30] of $T_1$. And it is not necessary for the Fermi level to be exactly on the anomaly for this to be active [31]. The detailed situations are nevertheless somewhat different in the various compounds.

In La$_{2-x}$Sr$_x$CuO$_4$, the maximum of $T_c$ occurs for $x \approx 0.16$, thus for a Fermi level far enough away from the mid band position of the Van Hove anomaly (corresponding to $x = 0$) to reduce $T_1$ by perhaps a factor 2 from its maximum value [31].
In YBa$_2$Cu$_3$O$_7$, the Van Hove anomalies should be split by two effects of similar amplitude:
- the orthorhombic distortion due to the CuO chains [14];
- the interference between the two CuO$_2$ planes due to $t'_\perp$ (cf. Appendix B).

As one does not know the exact number of electron carriers on the CuO chains and as there might be some holes in a more stable band, it is difficult to place the Fermi level accurately with respect to the van Hove anomalies. Preliminary positron annihilation studies suggest however that the Fermi level is sitting near to a van Hove anomaly [32], but further away from a van Hove anomaly of a second band. The splittings referred to above thus split the van Hove anomaly at least in two, thus decreasing $T_\perp$ by at least a factor two from its maximum value. The increase of $T_s$ with pressure confirms that the room pressure situation is not the optimum one.

In Bi and Tl compounds, the splitting due to the orthorhombic distortion does not exist; but that due to $t'_\perp$ remains and is even larger for $n = 3$. More details on the exact position of the Fermi level with respect to the van Hove anomalies are required to make a very detailed assessment of these cases.

In conclusion, the increase of the 3d magnetic or superconductive temperatures, roughly in proportion to the number of CuO$_2$ planes in each group in the new oxide superconductors, can be related to a stronger coupling between these planes, which reduces 2d fluctuations. Further increases in superconductive $T_c$ could be in principle obtained for still larger numbers $n$ of neighbouring CuO$_2$ planes in layered structures. But condition (8) limits practically $n$ to values less than typically 5, after which the meanfield temperature of order $T_\perp$ is obtained. It is also not yet completely clear, for such values of $n$, what are the best values of superconductive $T_c$ which avoid antiferromagnetism.

In this paper, we have assumed implicitly that the superconductive coupling occurs locally on the CuO$_2$ planes, and is a function of the local density of states on those planes. A hypothesis of spatially uniform density of states is on the contrary at the root of other interpretations of the variation of $T_c$ with $n$ [34, 35]. This last hypothesis does not seem to be physically grounded.

Acknowledgments.
The author wishes to thank J. Bok for discussions on this topic.

Appendix A.
Magnetic energy stored in a magnetic twist normal to the planes in a multiply layered structure.
The coupling magnetic energy reads, for the structure considered in the text,
\[
\varepsilon = \frac{1}{2} \sum_{i,j \text{ near to } i} J_{ij} S_i S_j = \frac{1}{2} \sum_{i,j \text{ near to } i} J_{ij} S^2 \cos (\phi_j - \phi_i) .
\]
In the elastic limit, this reads
\[
\varepsilon = \varepsilon_0 + \frac{1}{2} |J_{ij}| S^2 \frac{(\phi_j - \phi_i)^2}{2} .
\]

Consider a pure twist of $S_i$ with an axis $z$ normal to the $xy$ planes. $\phi_i$ only depends on $z$, i.e. on the rank $m$ of the $xy$ plane to which $S_i$ belongs. Then, if there are $N$ atoms per plane,
\[
\varepsilon = \varepsilon_0 + N \sum_m |J_{m,m+1}| S^2 (\phi_{m+1} - \phi_m)^2 .
\]
Equilibrium leads to
\[
\frac{1}{NS^2} \frac{d\varepsilon}{d\phi_m} = J_{m-1,m} (\phi_m - \phi_{m-1}) - J_{m,m+1} (\phi_{m+1} - \phi_m) = 0 . \quad (A.1)
\]
Hence the magnetic twist energy reads
\[
\varepsilon - \varepsilon_0 = NS^2 \left( \frac{1}{\sum_m |J_{m,m+1}|} \right) J_{0,1} (\phi_1 - \phi_0)^2 . \quad (A.2)
\]
For the layered structure considered in the text, condition (A.1) gives a twist $\delta \phi'_\perp$ between planes of a group which is smaller than the twist $\delta \phi_\perp$ between groups of planes, with
\[
J_\perp \delta \phi_\perp = J'_\perp \delta \phi'_\perp . \quad (A.3)
\]
If there are $n$ planes per group, equation (A.2) gives an average twist energy per atom.
\[
\left( \frac{n-1}{J_\perp} + \frac{1}{J'_\perp} \right) J_\perp S^2 \delta \phi_\perp^2 . \quad (A.4)
\]
As long as
\[
J'_\perp / J_\perp \gg n ,
\]
we see that the twist $(n-1) \delta \phi'_\perp$ within a group is negligible with respect to that $\delta \phi_\perp$ between groups, and the energy is concentrated between the groups. Each group behaves as a rigid unit in the twist along $z$. In consequence, it reacts as a single plane with interactions $J_\perp$ and $nJ_1$ in the $z$ and $xy$ directions respectively.

Appendix B.
Band structure of neighbouring CuO$_2$ planes in tight binding.
We consider two CuO$_2$ planes parallel to each other,
such that the Cu build square lattices and face each other in the two planes. We assume that the d\((x^2 - y^2)\) orbitals of each copper only interacts with the p orbitals of the 4 neighbouring oxygens and with the orbital of the opposite copper on the other plane. Thus, with obvious notations,

\[ H = H_0 + H'_0 + T'_\perp \left( |d_i\rangle \langle d'_i| + |d'_i\rangle \langle d_i| \right) \]

with

\[ H_0 = t_1 \sum_i \left[ |d_i\rangle \langle p_{x_i}| + |p_{x_i}\rangle \langle d_i| - |d_i\rangle \langle p_{y_i}| - |p_{y_i}\rangle \langle d_i| - |d_i\rangle \langle p_{x_{i-1}}| - |p_{x_{i-1}}\rangle \langle d_i| + |d_i\rangle \langle p_{y_{i-1}}| + |p_{y_{i-1}}\rangle \langle d_i| \right] + E_d \sum_i |d_i\rangle \langle d_i| + E_p \sum_i \left( |p_{x_i}\rangle \langle p_{x_i}| + |p_{y_i}\rangle \langle p_{y_i}| \right) \]

and a similar expression for \(H'_0\).

Taking

\[ |\psi\rangle = \sum_i e^{i k_\perp d_i} |d_i\rangle + d'|d'_i\rangle + p_x|p_{x_i}\rangle + p_y|p_{y_i}\rangle \]

the solution of \(H|\psi\rangle = E|\psi\rangle\) gives

\[ E = E_p \quad \text{(doubly degenerate)} \]

\[ E = \frac{1}{2} \left[ E_p + E_d \pm t'_\perp \pm \left( (E_d - E_p \pm t'_\perp)^2 + 4 t'^2 (|1 - e^{i k_\perp q}|^2 + |1 - e^{i k_\perp q}|^2) \right)^{1/2} \right]. \]

We see that the coupling \(t'_\perp\) only shifts the energy \(E_d\) by a small correction \(\pm t'_\perp\). In the reasonable limit where

\[ |t'_\perp| < |E_d - E_p| \]

the coupling \(t'_\perp\) only shifts the dp bands by an energy \(\pm t'_\perp\). This is clearly seen in band structure computation, from which one deduces

\[ |t'_\perp| \approx \frac{1}{10} t_1 \approx 0.1 \text{ eV}. \]

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[34] Grant, M., to be published (1988).