

Satellite peak ratios according to stripes theory

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(Dated: July 9, 2006)

This paper looks at the expected results for a neutron diffraction study according to stripes theory, paying attention to the ratio of incommensurate to satellite peaks. In particular this paper looks at a square wave profile for a crystal lattice and the effects of doping on the relative intensities of the peaks, for most doping levels seen in the literature (hole concentrations of $1/6 < p < 1/10$) it appears that in order to detect satellite peak phenomenon a good lower bound for the signal-to-noise ratio is around 10. Finally information on the signal-to-noise ratio along with the domain wall spacing and doping from some recent neutron diffraction experiments is presented, this gives the reader an idea of whether any satellite peaks are observable at present. Using the signal-to-noise ratio and comparing to the peak ratio, none of the experiments which were found could make a conclusive claim on the existence of satellite peaks.

I. INTRODUCTION

Inspired by recent neutron diffraction and low energy, inelastic neutron scattering experiments¹⁻³¹ a set of calculations has been done in order to see what predictions stripes theory makes concerning neutron diffraction experiments. Of particular interest is the ratio of the incommensurate peak to the largest satellite peak, as this will help interested parties evaluate the validity of arguments that the lack of observation of satellite peaks in neutron diffraction experiments invalidates stripes theory.

In order to do this it is important to establish a picture of the lattice which is being studied. The most basic model upon which everything else should be built is that of an undoped lattice, this structure is completely antiferromagnetic, meaning that the neighboring sites have opposite spin. As the lattice is doped with holes domain walls begin to appear, this can come in the form of taking place either on sites or bonds, the domain walls can form vertically or diagonally, finally the spacing between domain walls may vary.

While such a picture can present theoretical interest it should be testable. The results from this picture should be observable in neutron diffraction intensities because neutrons are affected by the magnetic properties of the lattice. It would then be possible to use the intensities to find the square of the Fourier transform of the lattice. For such diffraction experiments an undoped lattice yields a peak at the (π, π) point, as the material is doped with holes this peak is then split into multiple other peaks. The peaks with the largest intensities are referred to as incommensurate and the other peaks referred to as satellite peaks. The magnitudes and number of these satellite peaks are determined by the domain wall spacing and whether the domain wall is site-centered or bond-centered, though it appears that whether the domain wall is diagonal or vertical has no effect. As of yet no satellite peaks have been observed conclusively, however it is the focus of this paper to determine what the minimum signal-to-noise ratio is before one could reasonably expect to make such an observation and thus determine whether this lack of observation presents a problem

to stripes theory or if such a lack of observation is expected.

In order to see what exactly stripes theory predicts both the vertical and diagonal cases, as well as both the bond-centered and site-centered cases are considered. A general method for generating a model lattice and calculating the peak ratio for these parameters is given in Section II. The results of these calculations are presented in Section III. In Section IV the effects of doping on the satellite peak ratios are considered. Finally in Section V the doping, wall spacing, expected peak ratio and signal-to-noise ratio taken from some recent experiments are presented in order to evaluate the claim that satellite peaks should be visible.

II. MODEL

The model presented looks at the peak ratios if the spin distribution is approximated as a square wave. After creating a model lattice, the Fourier transform is taken and the peak ratio, defined in this paper as the ratio of intensities squared, between the incommensurate peak and the satellite peak is found. This represents the results from a neutron scattering study because:

$$S(\mathbf{Q})^{zz} = \frac{2\pi}{N} \sum_{\alpha} | \langle 0 | S_q^z | \alpha \rangle |^2 \delta(\omega - E_{\alpha}) \quad (1)$$

For neutron diffraction: $\delta(\omega - E_{\alpha})$ is only non-zero when $\alpha = 0$ which gives:

$$S(\mathbf{Q})^{zz} \propto | \langle S_q^z \rangle |^2 \quad (2)$$

which means that $S(\mathbf{Q})^{zz}$, seen in the neutron diffraction intensities is proportional to the squared Fourier transform of the lattice.^{32,33}

Three factors are taken into account, the first is whether the domain walls are site-centered or bond-centered, the second consideration is whether the wall stretches vertically or diagonally, and the final consideration is the spacing between domain walls. (For the

purposes of brevity only spacings of 2-5 are considered though in principle it is possible to use the model outlined for any spacing).

The first case considered is bond-centered, vertical stripes. (In the interest of clarity a convention of \tilde{j} has been used to substitute for j modulo a)

$$S_{i,j}^{VB}(a) = (-1)^i (-1)^j (-1)^{\frac{j-\tilde{j}}{a}} \quad (3)$$

Where a is the domain wall spacing. The i and j parts are due to the basic antiferromagnetism upon which this model is built. The $\frac{j-\tilde{j}}{a}$ represents the bond-centered domain wall. (See Figure 1)

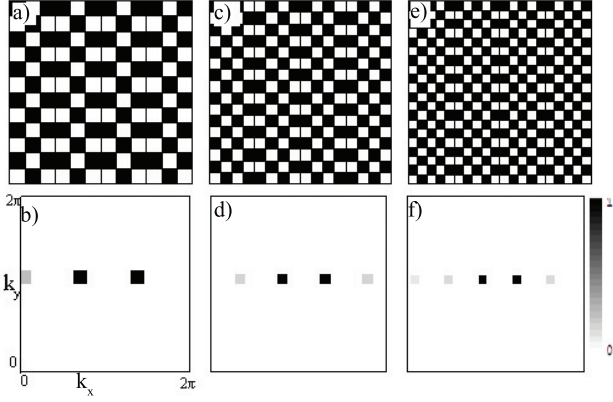


FIG. 1: Pattern for the vertical, bond-centered case. The left (a and b) represents a hole spacing of 3, the center (c and d) represents a spacing of 4 and the right (e and f) represents a spacing of 5. The spatial components are presented in a, c and e. The expected diffraction patterns are presented in b, d and f. From this diagram it is not difficult to distinguish satellite peaks for a spacing of 3 and 4, but it is a little difficult at a spacing of 5. It should be noted that for the satellite peaks the intensity is scaled is relative to the incommensurate peak.

For the vertical, site-centered case a multiplier is introduced to represent the lack of spin on the domain wall:

$$S_{i,j}^{VS}(a) = S_{i,j}^{VB}(a)(1 - \delta_{0,\tilde{j}}) \quad (4)$$

Next a diagonal geometry, such a pattern can be found in nickelates and at dopings between 0.02 and 0.05 for La based cuprates. (See Figures 3 and 4). This pattern is derived from the vertical case by changing j to $i + j$ for the domain wall factor, yielding:

$$S_{i,j}^{DB}(a) = (-1)^i (-1)^j (-1)^{\frac{(i+j)-(\tilde{i}+\tilde{j})}{a}} \quad (5)$$

For the diagonal, site-centered case a multiplier is introduced to represent a zero spin wall in the lattice:

$$S_{i,j}^{DS}(a) = S_{i,j}^{DB}(a)(1 - \delta_{0,\tilde{i}+\tilde{j}}) \quad (6)$$

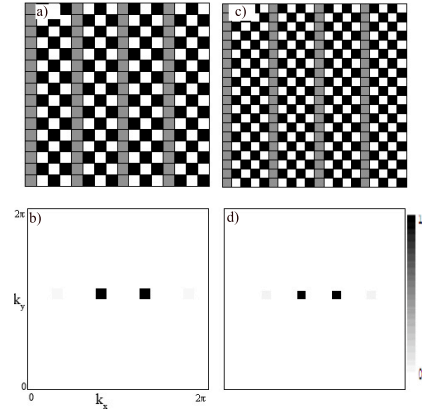


FIG. 2: Pattern for the vertical, site-centered case. The left (a and b) corresponds to a spacing of 4 and the right (c and d) to a spacing of 5. The spatial components are presented in a and c as well as the expected results from neutron diffraction in b and d. The satellite peaks are extremely difficult to distinguish from the background compared to the incommensurate peaks for this particular configuration. It should be noted that for the satellite peaks the intensity is scaled is relative to the incommensurate peak.

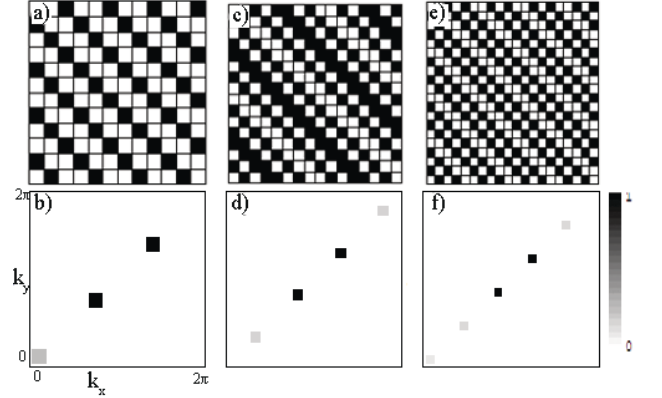


FIG. 3: Pattern for the diagonal, bond-centered case. The left (a and b) represents a hole spacing of 3, the center (c and d) represents a spacing of 4 and the right (e and f) represents a spacing of 5. The spatial components are presented in a, c and e also the corresponding results for neutron diffraction experiments are presented in b, d and f. For spacings of 3 and 4 the difference between the satellite peaks and background is slightly noticeable, however at a spacing of 5 such peaks are difficult to distinguish from the background. It should be noted that for the satellite peaks the intensity is scaled is relative to the incommensurate peak.

III. RESULTS

Because of these definitions the ratios of the incommensurate and satellite peaks are the same regardless of whether the domain wall stretches diagonally or vertically, thus for purposes of presenting numbers that particular datum is absent. Also a spacing of two is absent

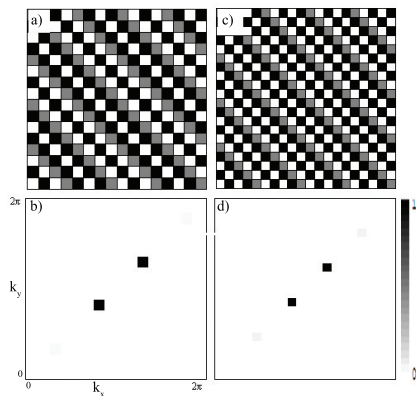


FIG. 4: Pattern for the diagonal site-centered case. The spatial components are presented in a and c while the neutron diffraction patterns are presented in b and d. In both of these cases the satellite peaks are nearly indistinguishable from the background. It should be noted that for the satellite peaks the intensity is scaled is relative to the incommensurate peak.

in all tables because that case has no satellite peaks. The results from these calculations can be found in Table I. Similar results for the site-centered case with a spacing of four were found by Tranquada *et al.* in³⁴

A diagram of the model lattices and the peak intensities as they would be observed by neutron scattering is presented in Fig. 1 for the vertical, bond-centered case, in Fig. 2 for the vertical, site-centered case, in Fig. 3 for the diagonal, bond-centered case and in Fig. 4 for the diagonal, site-centered case. In these diagrams black is used to represent the down spin, white is used to represent the up spin and gray is used to represent a site-centered hole in parts representing the real space of the lattice. In diagrams representing the results of neutron diffraction the intensities in all the diagrams are scaled relative to the incommensurate peak, with darker representing numbers closer to one and lighter representing numbers closer to zero.

For the site-centered case and higher spacings of the bond-centered case the satellite peaks are barely visible, which suggests that if the signal-to-noise ratio of an experimental instrument is not sufficiently large it will be difficult to detect such peaks. For the bond-centered case at lower spacings the satellite peaks are detectable, however at higher spacings (which are more likely to be encountered in experiments with cuprates) the satellite peaks are indistinguishable from background. The exact numbers for these calculations are given in Table I.

IV. THE EFFECTS OF DOPING

For the site-centered case regardless of the linear doping along the domain wall, the net spin is zero at that point. However, in the bond-centered case, doped holes along the domain wall are shared across at least the two

Location	Spacing	Peak Ratio
Bond	3	4.2
Bond	4	5.8
Bond	5	6.9
Site	3	∞
Site	4	34
Site	5	18

TABLE I: Results found for a square wave profile, as described in the text. It should be noted that the whether the domain wall is vertical or diagonal appears not to affect the peak ratios

sites neighboring the domain wall. This surely reduces the net spin on those sites. Therefore a new set of calculations is presented to determine the effects of doping on the peak ratio.

In order to determine the impact a quick calculation is done for the vertical, bond-centered case based on the 1/8 phenomenon where half of the vertical domain wall has a shared hole. In order to account for this both sites at the domain walls are adjusted to 3/4 based on the probability of hole placement. Such a simple modification gives rise to a change by a factor of approximately 2.5, clearly this phenomenon demands that it be taken in to account for a calculation to be anywhere near reasonable. Looking at the 1/8 phenomenon it is clear that given the incommensurability, δ , and the effective hole concentration, p , one can figure out the probability of any particular hole being present, then distribute this across the lattice to give rise to a model which takes in to account the linear doping along a domain wall. The mathematics behind this appears to be quite simple, first the incommensurability must be related to the domain wall spacing which is given as:

$$a = \frac{1}{2\delta} \quad (7)$$

Where a is the domain wall spacing and δ is the incommensurability. Next the probability for a particular hole being present must be found. As the hole concentration at a particular spacing, p_a , increases the number of holes found along the domain wall must also increase, therefore the probability must be proportional to the doping. As the domain wall spacing, a , increases the number of spaces for holes to be found in decreases therefore the probability must be proportional to domain wall spacing. Assuming that these are the dominant factors, and using the 1/8 phenomenon as normalizing point the following equation is obtained:

$$\text{Probability} = p_a a \quad (8)$$

Given the probability one can now split the probability of missing holes across the two sites and obtain:

$$S'_{i,j}{}^{VB}(a) = S_{i,j}^{VB}(a)[1 - (\delta_{0,\tilde{j}} + \delta_{1,\tilde{j}})\frac{p_a a}{2}] \quad (9)$$

and

$$S'_{i,j}{}^{DB}(a) = S_{i,j}^{DB}(a)[1 - (\delta_{0,i+\tilde{j}} + \delta_{1,i+\tilde{j}})\frac{p_a a}{2}] \quad (10)$$

Where p_a is the effective hole concentration for a particular domain wall spacing, a .

This paper uses values for the linear density of holes on the domain walls for LSCO using reference³⁵ and YBCO using reference³⁶, though in principle this method could be used for any metal oxide or adapted to new data given a similar curve to those found in the cited references. The results from calculations using this data are presented in Table II for LSCO and Table III for YBCO. As examples of what the lattices look like their images as well as their translated intensities are presented in Figures 5 (LSCO) and 6 (YBCO)

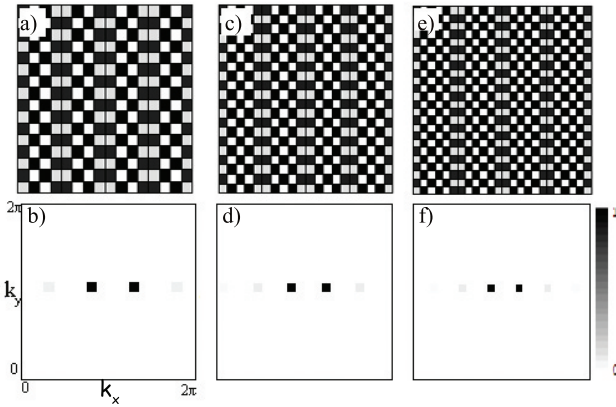


FIG. 5: LSCO: vertical, bond-centered case taking in to account doping. On the left (a and b) is a spacing of 4, in the center (c and d) 5 and on the right (e and f) 6. The spatial components are presented in a, c and e. The expected results from a neutron diffraction study can be found in b, d and f. The gray in the spatial components represents diminished spin. The satellite peaks are barely noticeable for this case, therefore it isn't difficult to imagine why such peaks may not be detectable.

From Tables II and III it appears clear that the bond-centered case still has the smallest ratio for normal dopings of LSCO and YBCO, however the peak ratios for such cases has increased. Also it appears that as a function of spacing the ratios now decrease as spacing increases. These results combined with those from Section III suggest that the effective hole concentration causes the peak ratios to diminish, this leads to the conclusion that the more interesting experiments will be those which have a higher spacing and lower dopings because these experiments approach the bare minimum prescribed in Section III, requiring a far lower signal-to-noise ratio.

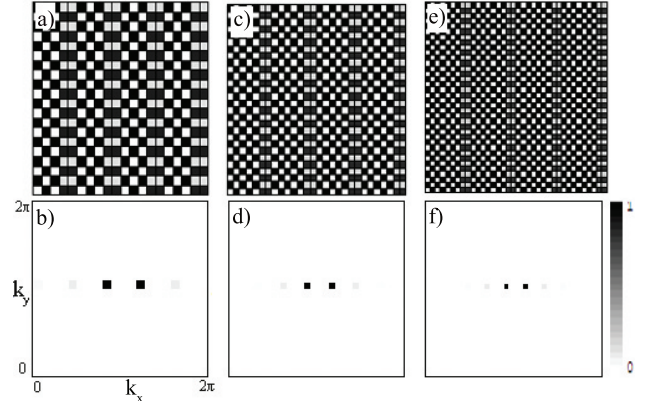


FIG. 6: YBCO: vertical, bond-centered case and taking in to account the effects of doping. On the left (a and b) is a spacing of 5, in the center (c and d) is a spacing of 7 and on the right (e and f) is a spacing of 9. The spatial components are presented in a, c and e, the neutron diffraction patterns can be found in b, d and f. The gray in the spatial components represents diminished spin. It should be quite easy to see why satellite peaks have yet to be detected as these diagrams show that compared to the incommensurate peaks they are barely distinguishable from background.

LSCO		
Location	Spacing	Peak Ratio
Bond	4	15
Bond	5	13
Bond	6	12

TABLE II: Results of calculations described in the second calculations section. It should be noted that because only the bond-centered case is affected that is what is presented. It should also be noted that for the spacing at three the hole concentration versus incommensurability appears to saturate for LSCO ($x > .18$).

V. DISCUSSION

It is suggested by some that the lack of observation of satellite peaks is a major weakness of stripes theory. These individuals point to a square wave profile as the spin wave and from this draw the conclusion that satellite peaks should be visible, however such broad statements should not be made lightly. The first point to consider is that such a statement is dubious at face value because such a profile hasn't been claimed by the stripes theory community. Ignoring this fact, assume for the sake of argument, as has been done in this paper, that it is the case that a square wave profile is prescribed by stripes theory. If one considers the site-centered case then the fact that no satellite peaks have been observed is not surprising at all as the greatest signal-to-noise ratio found, for a spacing greater than 3, is 12, which is too low to be able to see any satellite peaks. If the bond-centered

YBCO		
Location	Spacing	Peak Ratio
Bond	5	13
Bond	7	12.5
Bond	9	12

TABLE III: Results of calculations described in the second calculations section. It should be noted that for a domain wall spacing of four the hole concentration versus incommensurability appears to saturate for YBCO ($p > .1$).

case is considered then perhaps some concern is reasonable, according to the basic model satellite peaks should definitely be observable, however a square wave profile is unphysical in the bond-centered case and thus an objection based around such a model is groundless. When a more reasonable model, such as that presented in Section IV, is considered the ratio increases significantly, giving a ratio of 9 at minimum for large dopings, based on extrapolation from the bare minimum found in the square wave and a ratio above 12 for most spacings as seen in Table II for LSCO and Table III for YBCO. Given all of this one may point to the nickelate data presented in Table IV which has been taken with exemplary signal-to-noise ratios. The problem with the nickelate data is that the domain wall spacing is rather low ($2 < a < 5$) and the effective hole doping is rather high ($0.23 < p < 0.50$) these two facts suggest that the peak ratio is rather high. For example LNO with a spacing of 3 and an effective hole concentration of .26 the peak ratio is 54.

The calculations this paper presents are fairly rough as they grant assumptions which may not be the case such as a square wave profile in spite of the fact that many other configurations exist that lead to a peak ratio which is not as diminished. Real materials are certainly not as simple as a square wave profile and there is no doubt that other possible profiles exist that give a larger peak ratio, as this paper has found at least one method of finding such. The other assumption this model makes is on the width of the domain walls. For the bond-centered case it is assumed that the width of the wall is two sites wide and for the site-centered case it is assumed that the domain wall is one site wide, though it should be quite simple to expand the framework of this model so that the effects of different widths can be taken in to account.

The most important information presented in Table IV can be found in the hole doping, spacing, expected peak ratio and the signal-to-noise ratio, from these it should be clear whether a satellite, smaller peak should be observable in the presence of a large incommensurate peak. It should be noted that for all materials other than YBCO and LCO the expected peak ratio is calculated based on the doping and spacing. For YBCO the expected peak ratios are taken from Table III and for LCO the effective hole doping is found in the cited papers. Given that the data in the table is up to date, an absolute statement

can not yet be made on stripes theory. It is therefore suggested that more experiments need to be done especially in regions where there is a greater spacing between domain walls, as this is where the signal-to-noise ratio required to observe satellite peaks is the least.

Material	Doping	Spacing	Signal-to-Noise	Expected Peak Ratio	Ref.
LCO	.11	4	10	20-34	28
LCO	.12	4	7	20-34	29
LBCO	.125	4-5	7-9	15-34	2,21
LBSCO	.05	4	7	15-34	27
LSCO	.014	25	9	9.1-9.2	19
LSCO	.05	5-7	8-9	9.4-18	1,14,15
LSCO	.10	5	9	14-18	17
LSCO	.12	4	7-9	15-34	30,31
LSCO	.14	4	6	18-34	8
LSCO	.15	4	5-6	20-34	5,6,18
LSCO	.16	4	7-8	23-34	20
LSCO	.17	4	6	27-34	16
LSCO	.18	4	6	31-34	11
LSCO	.20	4	4	34-45	7,9
LSCO	.25	4	6	34-199	13
YBCO	0.5	5	3	13-18	12
YBCO	0.6	5-6	4-12	12.5-18	3,4,10
LNO	.13	3	23	54- ∞	22
LSNO	.23	5	10	18-89	24
LSNO	.27	4	8	34-700	23
LSNO	.33	3	15	23000- ∞	25
LSNO	.31	3	17	480- ∞	26

TABLE IV: Signal-to-noise ratio, doping and spacing are taken from various papers describing low energy inelastic neutron scattering and neutron diffraction experiments on cuprate superconductors. The doping in this table is x in $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$, $\text{La}_{1.875}\text{Ba}_{0.125-x}\text{Sr}_x\text{CuO}_4$, $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$, $\text{La}_2\text{CuO}_{4+x}$, $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$, $\text{La}_2\text{NiO}_{4+x}$, and $\text{La}_{2-x}\text{Sr}_x\text{NiO}_4$. The peak ratio ranges were calculated using both the site centered case and taking in to account the effects of doping for all spacings in the range provided.

VI. CONCLUSION

Overall a brief overview of calculations using a model lattice and the effects of doping on this model has been given. The main results can be found in Tables I, II, and III. In addition a method of obtaining more results is given allowing interested parties something to compare with. Data from recent experiments has been presented in Table IV and it appears that at the moment no conclusion can be made on stripes theory based on these experiments, therefore it is suggested more experiments are necessary so that a conclusive statement can be made.

Assuming that the signal-to-noise ratio is the same in all cases or that it does not drop as dramatically as the peak ratios, a possible region to focus on is where the spacing between domain walls is greatest as this is where the satellite peak tends to rise in proportion to the incommensurate peak therefore a signature, or lack thereof, is more likely to be found. Another place to look would

be the lightly doped, but region before the material becomes antiferromagnetic, in this region there are not as many holes to diminish the spin on sites adjacent to the bond-centered domain walls, this would be an area where the effects of doping are negligible and thus the first set of calculations, which has significantly lower peak ratios for most domain wall spacings, could be used.

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