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Phys. Rev. B **85**, 155130 — Published 17 April 2012

DOI: 10.1103/PhysRevB.85.155130

Observable NMR signal from circulating current order in YBCO

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(Dated: March 20, 2012)

Assuming, as suggested by recent neutron scattering experiments, that a broken symmetry state with orbital current order occurs in the pseudo-gap phase of the cuprate superconductors, we show that there must be associated equilibrium magnetic fields at various atomic sites in the unit cell, which should be detectable by NMR experiments.

I. INTRODUCTION

Varma[1] has proposed that the pseudogap state of the high temperature superconducting cuprates is a broken symmetry phase with equilibrium circulating currents within the unit cell as shown schematically in Figure 1. Indeed, recent polarized neutron scattering data[2–4] suggest that in at least some of the cuprates there is a phase transition at a pseudo-gap temperature, $T^\star > T_c$, to a state with a form of magnetic order which preserves the translational symmetries of the crystal. (Here T_c is the superconducting transition temperature and $T^\star$, determined from neutron scattering, is comparable to the previously determined pseudo-gap crossover temperature derived from transport and NMR studies.)

Specifically, the neutron scattering data suggest that there is some form of intra-unit-cell antiferromagnetic ordering in the pseudo-gap phase of underdoped YBCO and Hg1201 with ordered moments with magnitudes of order $0.1\mu_B$, tilted away from the c axis by a substantial angle (roughly $35^\circ - 65^\circ$). This is broadly compatible with the Varma loop order or with an alternative model (of a sort proposed by Fauque *et al.*[2]) with ordered moments on O sites.

Here, we determine the implications for Cu, Ba, and O NMR of the existence of magnetic symmetry breaking of the sort suggested by the neutron scattering experiments. We argue that the ordered moments observed in neutron scattering generically lead to magnetic fields of order $100G$ at the atomic sites, unless the field vanishes by symmetry. We will illustrate this with a symmetry analysis taking into account both the crystal structures and the neutron scattering data, from which we conclude that the likely ordered states do not posses sufficient symmetry to forbid fields at all the atomic sites. Finally, we will make an explicit calculation using the simplest physically plausible model of the distribution of currents within the unit cell (originally due to Weber *et al.*[5]). As expected, the resulting fields are large enough to be detectable. Though we present explicit calculations only for a specific model of orbital currents, we believe the conclusion is more general: any form of magnetic order consistent with the observed neutron scattering in Hg-1201 and YBCO will lead to large magnetic fields at most atomic sites.

II. PRELIMINARY ESTIMATE AND SYMMETRY CONSIDERATIONS

To estimate the order of magnitude of the expected fields, we consider a circular current loop of dipole moment μ and radius r. The field at the center has strength

$$B(\mu, r) = \frac{2\mu}{cr^3} = 325G \left(\frac{\mu}{\mu_B}\right) \left(\frac{a}{r}\right)^3,$$

where $a = 3.8$Åis the Cu-Cu distance. Taking $r = \frac{a}{2}$ and $\mu = 0.1\mu_B$ (as reported by Mook *et al.*[3]), this gives $B = 260G$.

We now briefly review the symmetry considerations governing the existence of a static (thermodynamic) magnetic field, $\vec{B}(\vec{r})$ at any given position in the unit cell of a crystal. Specifically, if certain symmetries are preserved, it is possible to prove that the magnetic field vanishes. If the field does not vanish by symmetry, the likely implication is that the field is non-zero.

Let $\mathcal{G}_{\vec{r}}$ be the set of point group symmetry operations in the considered state of the system which leave the spatial point $\vec{r}$ invariant. If there exists any group element $g \in \mathcal{G}_{\vec{r}}$, such that g transforms $B_a(\vec{r}) \to -B_a(\vec{r})$, it follows that $B_a(\vec{r}) = 0$.

Since $\vec{B}$ is odd under time-reversal (T), if time-reversal symmetry is unbroken, then $\vec{B}(\vec{r}) = 0$ for all $\vec{r}$. However, if time-reversal symmetry is broken, the field may still vanish at points of sufficiently high symmetry. The Varma state breaks both time-reversal and rotation by π (R_π) about a line parallel to the c axis and passing through any atomic site, but preserves the product of these (TR_π). Since TR_π transforms $B_c \to -B_c$, the out-of-plane component of the magnetic field must vanish at all atomic sites for both Hg-1201 and YBCO.

Because $\vec{B}$ is a pseudo-vector, any component of $\vec{B}$ that lies in a mirror plane is odd under reflection through this plane. Thus, if there is a symmetry with respect to a reflection plane passing through point $\vec{r}$, then all components of $\vec{B}(\vec{r})$ within that plane must vanish. We will assume that the loop order leaves unbroken the reflection symmetry about the Cu-O plane in Hg-1201, and about the Y plane in YBCO, both of which we term M. Along with TR_π symmetry, this assures that there is no net ferromagnetism in the loop ordered state. This reflection symmetry also implies that the in-plane components of the magnetic field vanish in the Cu-O plane of Hg-1201.

Finally, to simplify the discussion, we will assume the existence of an additional unbroken reflection symmetry D about a diagonal plane containing the Cu, apical O, and Ba sites in both materials. This is at best approximate in YBCO, which

is orthorhombic in the normal state, and thus would be monoclinic in the Varma state. However, since the YBCO lattice is tetragonal to within 2%, deviations from this symmetry are likely to be small. Note that to the extent that the actual ordered state in question breaks further symmetries, there is still stronger reasons to expect detectable magnetic fields at the various nuclear sites.

In summary, if there exists a Varma loop ordered state in Hg-1201 or YBCO, the M and TR_π symmetries require $\vec{B}(\vec{r})$ to vanish at the Cu and planar O sites. However, non-vanishing fields parallel to the Cu-O plane are permitted by symmetry at the apical O and Ba sites of Hg1201, and at the Ba, Cu, apical O, and planar O sites of YBCO. The D reflection symmetry further constrains the directions of the fields. For instance, in Hg-1201, the field at the apical O and Ba sites must point along a unit cell diagonal. (Note that similar symmetry considerations applied to the d-density wave state[6] imply vanishing magnetic fields at the Cu and all the O sites in Hg-1201 and at the Cu, and apical O sites in YBCO, but permit an in-plane magnetic field at the in-plane O sites in YBCO, and an out-of-plane magnetic field at the Ba sites of both Hg-1201 and YBCO.)

III. EXPLICIT MODEL

For simplicity, we consider a model in which only the Cu-O planes are electronically active, and in which we ignore the orthorhombicity of the YBCO lattice and any small buckling of the in-plane O-Cu-O bond. We assume the symmetries mentioned in the previous section as well as lattice translation symmetry.

The ideal two dimensional cartoon of the state originally proposed by Varma is sketched in Figure 1. Since in the cuprates, the distance to the apical O is comparable to the distance between planar O's, we must take into account currents involving the apical O, even if we take the simplest (shortest-range) version of this state adapted to the actual materials. (This was recognized previously in Refs.[3,4,7], as it is necessary to account for the presence of the in-plane components of the magnetic order inferred from the neutron scattering experiments.) The assumption of near-neighbor currents and the symmetries previously assumed lead to the pattern of currents shown in Figures 2 and 3 for YBCO and Hg 1201, respectively. Note that TR_π symmetry forbids a current between the apical O and Cu sites, while the reflection symmetries M and D ensure that the precise pattern of broken symmetry in the proposed state is defined by the three independent currents labeled I_j in the figures.

The model presented (originally described by Weber *et al.*[5]) is broadly consistent with the neutron scattering data in that it would result in magnetic scattering intensity at suitable Bragg vectors with a polarization dependence reflecting comparable strengths of the in-plane and out-of-plane magnetic fields (see Appendix B for more details). However, there is at least one unresolved discrepancy: The in-plane component of the magnetization at (010) must vanish so long as M is unbroken. Experimental data[3] indicate a tilted moment at (010), though this is only reported for one experiment in the published literature, and with a substantial stated margin of error.

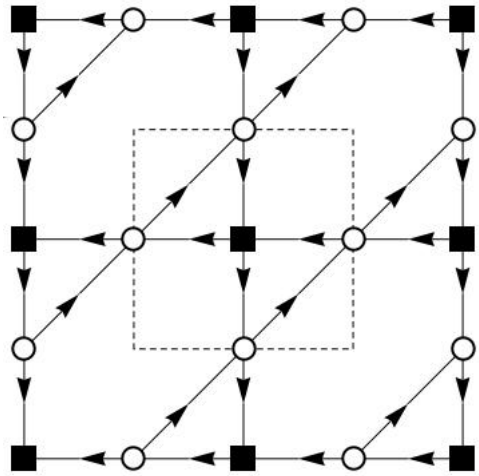

Figure 1: Top view of circulating currents in the Varma loop ordered state. Cu sites are black rectangles, O sites white circles.

Before making a quantitative comparison with experiment, we have imposed the additional constraint, not required by symmetry, that there be no net current flowing through the system in equilibrium. This is equivalent to taking $I_3 = I_1 + I_2$ in Figures 2 and 3. Assuming that "form factor" effects associated with the spatial extent of these currents can be neglected, the resulting magnetic field that would be produced by this state can be directly computed (as sketched in the Appendix) in terms of the two remaining independent parameters I_1 and I_2. These can be determined by comparing the measured and predicted spin-flip magnetic scattering cross-sections for orthogonal neutron polarizations at a single Bragg wave-vector. For both YBCO and Hg-120, the most studied Bragg peak is (011), so we determine the values of I_j for each material using data from that peak only. Since the scattering cross-section is quadratic in the currents, there are two independent solutions for I_1 and I_2. Naturally, once the currents are determined, it is straightforward to compute the field at any particular spatial point. We quote results for each of the two independent solutions for I_1 and I_2.

IV. RESULTS AND DISCUSSION

For the case studied in Ref.[3] of $YBa_2C_3O_{6+\delta}$ with $\delta = 0.6$ and $T_c = 61K$, the analysis described above leads to the prediction of fields of 100's of G at various sites in the unit cell, consistent with the dimensional estimate presented above. In particular, we predict fields of $700G$ or $710G$ at the copper site, $230G$ or $130G$ at the barium site, $170G$ or $280G$ at the apical oxygen sites, and $360G$ or $350G$ at the in-plane oxygen sites. Additional symmetries in Hg1201 lead to quite different results. In particular, as required by symmetry, the fields at both the Cu and the planar O sites vanish exactly. However, if we apply the present analysis to the neutron data of Ref.[4] for underdoped Hg 1201 ($T_C = 81K$), we infer that at

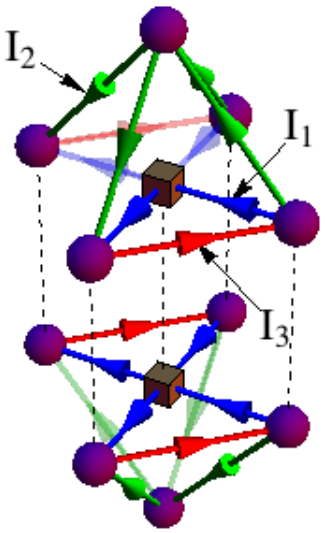

Figure 2: Microscopic model for YBCO. O sites are spheres, Cu sites are cubes.

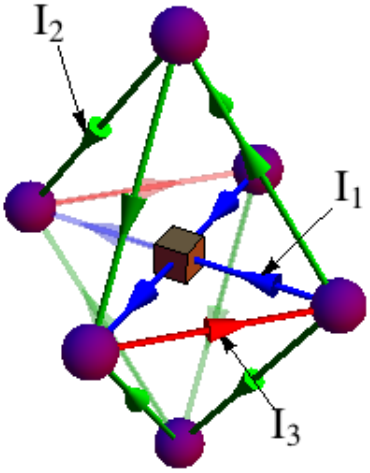

Figure 3: Microscopic model for Hg1201. O sites are spheres, Cu sites are cubes.

low temperatures there should be a field of $180G$ or $200G$ at the apical oxygen site, and $240G$ or $170G$ at the Barium site. Observed[8] Cu NMR line-widths in YBCO are of order 100G and O linewidths substantially smaller, so these effects should be readily observable.

There are, of course, uncertainties in the quantitative estimates we have made associated with the error bars on the neutron data. As previously mentioned, the assumed pattern of currents is also not fully consistent with the neutron data because the latter show a small tilt angle at (010) which the symmetries of the model state forbid. Some quantitative changes could arise from form factors associated with the non-zero spatial extent of the equilibrium currents, and with currents flowing between further neighbor sites in the lattice. We do not believe, but have not proven, that these uncertainties will cause qualitative revisions in the estimates we have made. We have also treated the currents classically, which is a valid procedure in typical situations involving broken symmetry states. However, He and Varma[9] have argued that there is an essentially quantum character to the loop ordered state which invalidates such an approach. Finally, a magnetic ordering that appears static within the frequency resolution of neutron scattering may be rapidly fluctuating on NMR timescales. Though no obvious mechanism exists for an order fluctuating on intermediate timescales, it would be consistent with the neutron results and the symmetries assumed, yet yield a null result in NMR experiments. In any case, the presence of static magnetic fields at the various atomic sites in the crystals, if seen, would constitute strong evidence of the putative current loop order in the pseudo-gap phase of these materials.

At present, we are unable to find published Cu or O NMR studies which give clear results concerning the existence or absence of fields of the predicted magnitude in YBCO or Hg1201. Work by Strässle *et al.*[10] sets an upper bound of less than $1G$ for the field at the Barium site of YBCO 248. However, since neutron scattering is not available for this material, this bound cannot be directly compared with a predicted magnitude. We hope that the results in this Brief Report will encourage experimental tests of local magnetic fields in the pseudogap state of the aforementioned materials.

Acknowledgements: We thank C. Varma and P. Bourges for helpful comments. This work was supported in part by DOE Grant No. AC02-76SF00515 at Stanford.

V. APPENDIX A: SKETCH OF CALCULATIONS

The neutron scattering data used in these calculations are the cross sections for elastic magnetic neutron scattering in the spin-flip channel for two independent polarizations. The Born approximation gives the differential scattering cross section at momentum transfer $\vec{K}$ (a reciprocal lattice vector) as

$$I_{\hat{P}}(\vec{K}) = \left(\frac{m_N}{2\pi\hbar^2}\right)^2 \left(\frac{g\mu_N}{2}\right)^2 \left|\vec{B}_{\vec{K}} - \hat{P}\left(\hat{P}\cdot\vec{B}_{\vec{K}}\right)\right|^2$$

where $g = -3.826$ is the neutron g-factor, μ_N the nuclear magneton, $\hat{P}$ the polarization direction of the incoming neutrons, and $\vec{B}_{\vec{K}}$ is the Fourier transform of the magnetic field. The momentum transfer $\vec{K}$ employed in Refs[2–4] is (011). The magnetic field component at this wavevector can be expressed in terms of the currents I_1, I_2, and I_3 as

$$\vec{B}_{\vec{K}} = -\frac{4\pi i}{c}\frac{\vec{K}\times\vec{J}_{\vec{K}}}{K^2}$$

where $\vec{K}$ is a reciprocal lattice vector, and the current density $\vec{J}_{\vec{K}}$ can be expressed as

$$\vec{J}_{\vec{K}} = -2\sum_n I_{j_n}\hat{e}_n \frac{\sin\left(\vec{K}\cdot\hat{e}_n\frac{L_n}{2}\right)}{\vec{K}\cdot\hat{e}_n} e^{i\vec{K}\cdot\vec{\mathcal{R}}_n}.$$

Peak	σ_{theory}	σ_{exp}	$(\sigma_z/\sigma)_{theory}$	$(\sigma_z/\sigma)_{exp}$
(011)	1.6	1.6 ± 0.2 (UD61)	0.66	0.6 ± 0.2 (UD61)
(010)	7.2	8.0 ± 1.0 (UD54)	1	0.8 ± 0.2 (UD63)
(012)	1.0	0.2 ± 0.2 (UD54)	0.99	not reported
(002)	1.3	0 (UD54)	0.5	undefined
(021)	0.3	0 (UD63)	1	undefined

Table I: Comparison of model to available neutron scattering data for YBCO. Scattering cross sections are given in millibarns. The current parameters of the model were chosen to fit the peak most extensively studied, (011). Data for the UD61and UD54 samples is from Sidis *et al.*[11], UD63 is from Mook *et al.*[3]. σ_z is the cross section for magnetic spin-flip scattering for an initial neutron polarization perpendicular to both the momentum transfer and the scattering plane (i.e. polarization along (100) for these peaks). The ratio σ_z/σ maps directly to the tilt angle, so that when the ratio is one, the effective moment lies along the c axis.

In this expression the sum runs over the current-carrying bonds (segments) in a unit cell. For a given segment n, I_{j_n} is the current (I_1, I_2, or I_3, as defined previously), $\hat{e}_n$ is the direction of current flow, L_n is the length of the bond, and $\vec{\mathcal{R}}_n$ is the position of the bond midpoint.

With these results, we can write the scattering cross section as a function of the currents, and then invert to solve for these currents in terms of the experimental data. We then evaluate the real space magnetic field using the Biot Savart Law. All told, the field is

$$\vec{B}(\vec{r}) = \sum_{\vec{R}} \sum_{n} \frac{I_{j_n}}{c} \frac{\vec{a} \times \hat{e}_n}{|\vec{a} - (\hat{e}_n \cdot \vec{a})\hat{e}_n|^2} \cdot \left(\frac{\vec{a} \cdot \vec{e}_n + \frac{L_n}{2}}{|\vec{a} + \frac{L_n}{2}\vec{e}_n|} - \frac{\vec{a} \cdot \vec{e}_n - \frac{L_n}{2}}{|\vec{a} - \frac{L_n}{2}\vec{e}_n|} \right)$$

In this expression the first sum runs over all unit cells of the crystal (i.e. $\vec{R}$ runs over all Bravais lattice vectors), the second sum is over the current-carrying bonds in a unit cell as above, and the position of a given segment is $\vec{a} \equiv \vec{a}_{n,\vec{R}} = \vec{R} - \vec{r} + \vec{\mathcal{R}}_n$. The sum converges rapidly.

VI. APPENDIX B: COMPARISON OF MODEL TO DATA

The explicit model used for calculation is intended only as an example, but nonetheless is in qualitative agreement with the published elastic neutron scattering data, as shown in Table I. Note, however, that the data at different Bragg peaks come from different crystals with substantially different T_c's, and so are not directly comparable. The assumption of reflection symmetry about the Y plane requires that the ordered moment point along the c axis for all Bragg peaks (H,K,2L). Accordingly the model cannot reproduce the small tilt moment reported at (010) in YBCO, though this appears to be within the margin of error of the experiment. If we no longer assume reflection symmetry about the Yttrium plane, the model can accommodate the tilt at (010), but this requires fine tuning of parameters to avoid ferromagnetism. Since the tilt angle is small, the predicted magnetic fields are qualitatively similar.

In addition, the predicted cross sections substantially exceed those measured for the higher order peaks. This disagreement could simply be due to a form factor reflecting the spatial spread of the physical currents; the model assumes line currents (i.e. neglects form factors).

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