Magnetic field-induced soft mode in spin-gapped high-\(T_c\) superconductors

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We present an explanation of the dynamical in-gap spin mode in La\(_{2-y}\)Sr\(_y\)CuO\(_4\) (LSCO) induced by an applied magnetic field \(H\) as recently observed by J. Chang et al\(^{13}\). Our model consists of a phenomenological spin-only Hamiltonian, and the softening of the spin mode is caused by vortex pinning of dynamical stripe fluctuations which we model by a local ordering of the exchange interactions. The spin gap vanishes experimentally around \(H = 7\)T which in our scenario corresponds to the field required for overlapping vortex regions.

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The cuprate superconductors (SC) arise from doping an antiferromagnetic (AF) Mott insulator. At half-filling the spin spectrum of La\(_2\)CuO\(_4\) is quantitatively described by a spin-1/2 Heisenberg model.\(^2\) At finite doping, however, the nature of the magnetic fluctuations and their importance for SC remains controversial. At present, the so-called "hour-glass" dispersion observed in inelastic neutron response appears universal whereas details of the low-energy spin fluctuations vary between the compounds.\(^2\) In the optimal and overdoped regimes an interplay between magnetism and SC has been revealed by the opening of a spin gap which scales with the SC transition temperature \(T_c\). This is in contrast to the underdoped regime where LSCO and Bi\(_2\)Sr\(_2\)CaCu\(_2\)O\(_{8+\delta}\) (BSCO) are known to exhibit spin freezing well into the SC dome\(^{15,16}\) whereas YBa\(_2\)Cu\(_3\)O\(_{6+x}\) (YBCO) reveals a static signal only at very low doping.\(^8\)

In the quest of obtaining a better understanding of these materials, the effect of an applied magnetic field \(H\) has been extensively used, also in neutron scattering experiments. In the underdoped regime a magnetic field applied perpendicular to the CuO\(_2\) planes enhances static incommensurate (IC) stripe order, which exist at \(H = 0\) presumably due to impurities.\(^9,11\) This enhanced signal at the IC positions \(q^*\) [quartet of peaks near \((\pi, \pi)\)] has been seen both in underdoped La\(_{2-y}\)Sr\(_y\)CuO\(_4\)\(^{9,12,13}\) La\(_2\)CuO\(_4+y\)\(^{14}\) and very recently also in YBa\(_2\)Cu\(_3\)O\(_{6+\delta}\).\(^5\) A similar enhancement of stripe order can be obtained at \(H = 0\) by the use of impurity substitution.\(^15,16,17,18\) Furthermore, experiments have shown that spin-gapped samples can transition from a SC phase to a coexisting SC and IC stripe ordered phase by use of a magnetic field.\(^13,19\)

In LSCO, static order is absent for doping levels beyond approximately \(x \sim 0.13\).\(^5\) The inelastic spin excitations are, however, still characterized at low energy by the same IC wavevectors but a spin gap of order \(\sim 3-7\) meV develops at \(T < T_c\).\(^20,21,22,23\) The \(H\)-dependence of the low-energy inelastic neutron response has also been subject of intense experimental investigations. Lake et al.\(^{24}\) reported a softening of the spin mode in LSCO \((x = 0.163)\) revealed by an in-gap mode observed with \(H = 7.5\)T compared to a fully spin-gapped spectrum for \(H = 0\). Similar results have been obtained at larger doping levels.\(^25,26\) More recently detailed inelastic neutron scattering experiments studied the \(H\)-dependence of the magnetic spin gap in slightly underdoped LSCO \((x = 0.145)\).\(^1\) At this doping, a critical field of \(H_c = 7\)T is required to tune the system from a SC state into a phase with coexisting SC and long-range IC stripe order. At applied fields \(0 < H < 7\)T the spin gap is diminished and an in-gap spin mode is observed.\(^1,24\) This transition is very reminiscent of the dynamic neutron response seen e.g. by Kimura et al.\(^{16}\) in Zn-doped LSCO \((x = 0.15)\).

The presence of SC regions appear important for the existence of enhanced magnetic response at these relatively low applied fields \(H \sim 0 - 10\)T; only when vortices can act as additional pinning centers for nucleation of stripe regions do they lead to an enhanced magnetic response. This agrees qualitatively with: 1) the fact that the enhanced signal is seen at \(T < T_c\), and 2) an absent [a negligible] magnetic field effect in non-SC [weakly SC] samples.\(^27,28,29\) It is not necessary for the vortices to form an ordered lattice which also appear absent at \(x = 1/8\) in LSCO.\(^1\) Theoretically, the existence of AF order induced by vortices was first discussed within the SO(5) theory of the cuprates.\(^30,31,32\) Later several models studied how vortices may nucleate magnetic regions due to a general competition between SC and stripe order.\(^33,34,35,36,37,38,39\)

One way to model the stripe phase is in terms of coupled spin ladders.\(^40,41,42,43,44,45\) In such spin-only models, the charge carriers are assumed important only for renormalizing the exchange couplings between localized spinful regions, and the Hamiltonian is of the Heisenberg form. Clearly this approach is phenomenological, and should be considered an approximate effective model. Nevertheless, this approach has been very successful is describing e.g. the universal "hour-glass" magnetic dispersion.

Here, motivated by the recent experimental findings of Chang et al.\(^{13}\) we study theoretically the effect of a magnetic field on the low-energy (gapped) spin fluctuations. By extending the coupled spin ladder approach to include the effect of vortices, we find a field-induced mode inside...
the primary effect of a magnetic field is to introduce vor-
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tex regions of ordered stripes where all the inter-ladder bonds have strength $J_{v}^{\text{inter}} = -0.6J$. The motivation for this effective "exchange-ordering" nature of $H$ comes from recent quantum oscillation measurements which indicate that an external magnetic field cause exactly this kind of ordering of the stripes resulting in a severe Fermi surface reconstruction.

In order to find the spin excitation spectra we simulated Heisenberg spin systems as depicted in Fig. 1 at a temperature $T = 0.01J$ using the quantum Monte Carlo stochastic series expansion technique with directed-loop updates. This technique yields high quality results for the imaginary-time correlation function which is continued to real frequencies using the Average Spectrum Method where the average over all possible spectra is taken weighted by how well each spectrum fits the data. This approach performs at least as well as MaxEnt methods for high quality imaginary-time data.

The bulk part $S_b(q^*, \omega)$ and the vortex part $S_v(q^*, \omega)$ of the structure factor were simulated separately. For the bulk we diluted the arrangement of $J_{b}^{\text{inter}}$ bonds randomly prior to performing the simulations. The structure factor $S_b(q^*, \omega)$ was extracted for each disorder realization and the average was taken. With an interladder bond dilution fraction of 30% we found that $S_b(q^*, \omega)$ has a sharp peak around $\omega = 0.1J$ as well as a broader high energy peak at $\omega = 0.2J$ as seen from the inset in Fig. 2. This two-peak structure at the IC position $q^*$ is consistent with inelastic neutron scattering measurements on spin-gapped LSCO. Without a microscopic model including realistic disorder concentrations it is hard to estimate the correct degree of bond disorder within the present spin-only approach. However, the position of the low energy peak depends on the amount of bond dilution,
order 10% of less dilution moves the peak down in energy, and we have simply chosen 30% in order to reproduce a spin gap of order 10% of $J$ as reported in Ref. [1].

For the vortex regions we use the non-diluted configuration to obtain $S_v(q^*, \omega)$ which has a structure similar to Fig. 2 except that the low-energy peak has moved further down in energy. For $J_{\text{inter}}^v = -0.6J$, the lowest peak is roughly at $\omega = 0.02J$ (see Fig. 3). This corresponds to $\omega \sim 2\text{meV}$ in agreement with Ref. [1] using recent estimates for the exchange coupling $J \sim 100\text{meV}$ in LSCO ($x = 0.14$). The peak position is dependent on both the finite size of the vortex region and the value of $J_{\text{inter}}^v$; as expected smaller vortex regions (or smaller value of $|J_{\text{inter}}^v|$) moves the peak upwards in energy. Taking into account that for $H = 2.5T$ (as used in Ref. [1]) the bulk region contributes roughly 15 times more to the total $S(q^*, \omega)$ than the vortex regions, we compose the total structure factor $S(q^*, \omega) = (15S_v(q^*, \omega) + S_c(q^*, \omega))/16$ shown in Fig. 3. As seen, $H$ induces an in-gap mode similar to the experimental results of Refs. [1] and [2].

At low magnetic fields [$H \lesssim 3T$ in LSCO ($x = 0.145$)], an increase of $H$ enhances the vortex density, but the size of each vortex region is presumably unchanged resulting in a fixed energy of the in-gap spin mode. In this field range the spectral weight of the in-gap mode should increase as a consequence of an increased weighting of the total structure factor by the denser amount of vortex regions. By contrast when vortex regions overlap, the mode will rapidly move to zero energy becoming a true Bragg signal. Vortex regions of size $\sim 100\text{Å}$ will start overlapping at $H \sim 6T$ in agreement with the closing of the spin gap found in Ref. [1] near this field strength. Theoretically, the generation of a Bragg peak happens if $J_{\text{inter}}^v$ is larger than the critical value $J_{\text{inter}}^c$ needed for long-range stripe order. By contrast, if $|J_{\text{inter}}^v| < |J_{\text{inter}}^c|$, a finite energy peak can still show up at finite field, but it will not move to zero as the vortex regions start overlapping.

In conclusion we have proposed an explanation for the soft magnetic mode observed inside the spin gap of LSCO in terms of magnetic field-induced stripe ordered vortex regions. At zero applied magnetic field $H = 0$ the CuO$_2$ planes are modeled as disordered coupled spin ladders known to reproduce the magnetic "hour-glass" dispersion seen by experiments. At finite field $H \neq 0$ vortices are simulated by regions of ordered exchange couplings. Our calculation shows that stripe pinning by vortices gives a consistent picture of the in-gap spin mode observed in recent inelastic neutron scattering measurements.

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1. J. Chang, N. B. Christensen, Ch. Niedermayer, K. Lefmann, H. M. Ronnow, D. F. McMorrow, A. Schneiderwind, P. Link, A. Hiess, M. Boehm, R. Mottl, S. Pailhés, N. Momono, M. Oda, M. Ido, and J. Mesot, arXiv:0902.1191v1.

2. R. Coldea, S. M. Hayden, G. Aeppli, T. G. Perring, C. D. Frost, T. E. Mason, S.-W. Cheong, and Z. Fisk, Phys. Rev. Lett. 86, 5377 (2001).
Rønnow, B. Lake, C. D. Frost, and T. G. Perring. Nature Phys. 3, 163 (2007).