科技资料

Dynamics of Magnetic Fluctuations in High-Temperature Superconductors

Dynamics of Magnetic Fluctuations in High-Temperature Superconductors

Edited by

George Reiter

University of Houston
Houston, Texas

Peter Horsch

Max-Planck-Institut für Festkörperforschung
Stuttgart, Germany

and

Gregory C. Psaltakis

University of Crete
and Research Center of Crete
Heraklion, Greece

Plenum Press
New York and London
Published in cooperation with NATO Scientific Affairs Division

Proceedings of a NATO Advanced Research Workshop on
Dynamics of Magnetic Fluctuations in High-Temperature Superconductors,
held October 9-14, 1989,
in Aghia Pelaghia, Crete, Greece

Library of Congress Cataloging-in-Publication Data

NATO Advanced Research Workshop on Dynamics of Magnetic Fluctuations in High-Temperature Superconductors (1989 : Hagia Pelagia, Greece)
Dynamics of magnetic fluctuations in high-temperature superconductors / edited by George Reiter, Peter Horsch, and Gregory C. Psaltakis.
p. cm. -- (NATO ASI series. Series B, Physics ; v. 246)
"Proceedings of a NATO Advanced Research Workshop on Dynamics of Magnetic Fluctuations in High-Temperature Superconductors, held October 9-14, 1989, in Aghia Pelaghia, Crete"--T.p. verso.
"Held within the program of activities of the NATO Special Program on Condensed Systems of Low Dimensionality, running from 1983 to 1988 as part of the activities of the NATO Science Committee"--
"Published in cooperation with NATO Scientific Affairs Division."
Includes bibliographical references and index.
ISBN 0-306-43810-0
1. High temperature superconductors--Congresses. 2. Valence fluctuations--Congresses. I. Reiter, George. II. Horsch, Peter. III. Psaltakis, Gregory C. IV. North Atlantic Treaty Organization. Scientific Affairs Division. V. Special Program on Condensed Systems of Low Dimensionality (NATO) VI. Title. VII. Title: Magnetic Fluctuations in High-Temperature Superconductors. VIII. Series.
QC611.98.H54N36 1989
537.6'23--dc20 91-10370
CIP

Printed in the United States of America

SPECIAL PROGRAM ON CONDENSED SYSTEMS OF LOW DIMENSIONALITY

This book contains the proceedings of a NATO Advanced Research Workshop held within the program of activities of the NATO Special Program on Condensed Systems of Low Dimensionality, running from 1985 to 1990 as part of the activities of the NATO Science Committee.

Other books previously published as a result of the activities of the Special Program are:

Volume 148 INTERCALATION IN LAYERED MATERIALS
edited by M. S. Dresselhaus

Volume 152 OPTICAL PROPERTIES OF NARROW-GAP LOW-DIMENSIONAL STRUCTURES
edited by C. M. Sotomayor Torres, J. C. Portal, J. C. Maan, and R. A. Stradling

Volume 163 THIN FILM GROWTH TECHNIQUES FOR LOW-DIMENSIONAL STRUCTURES
edited by R. F. C. Farrow, S. S. P. Parkin, P. J. Dobson, J. H. Neave, and A. S. Arrott

Volume 168 ORGANIC AND INORGANIC LOW-DIMENSIONAL CRYSTALLINE MATERIALS
edited by Pierre Delhaes and Marc Drillon

Volume 172 CHEMICAL PHYSICS OF INTERCALATION
edited by A. P. Legrand and S. Flandrois

Volume 182 PHYSICS, FABRICATION, AND APPLICATIONS OF MULTILAYERED STRUCTURES
edited by P. Dhez and C. Weisbuch

Volume 183 PROPERTIES OF IMPURITY STATES IN SUPERLATTICE SEMICONDUCTORS
edited by C. Y. Fong, Inder P. Batra, and S. Ciraci

Volume 188 REFLECTION HIGH-ENERGY ELECTRON DIFFRACTION AND REFLECTION ELECTRON IMAGING OF SURFACES
edited by P. K. Larsen and P. J. Dobson

Volume 189 BAND STRUCTURE ENGINEERING IN SEMICONDUCTOR MICROSTRUCTURES
edited by R. A. Abram and M. Jaros

Volume 194 OPTICAL SWITCHING IN LOW-DIMENSIONAL SYSTEMS
edited by H. Haug and L. Banyai

Volume 195 METALLIZATION AND METAL–SEMICONDUCTOR INTERFACES
edited by Inder P. Batra

Volume 198 MECHANISMS OF REACTIONS OF ORGANOMETALLIC COMPOUNDS WITH SURFACES
edited by D. J. Cole-Hamilton and J. O. Williams

SPECIAL PROGRAM ON CONDENSED SYSTEMS OF LOW DIMENSIONALITY

PREFACE

This NATO Advanced Research Workshop was held at a time when there was little consensus as to the mechanism for high temperature superconductivity, in the context of a world undergoing major changes in its political alignments and sense of the possibility for the future. It was characterized by generosity in the sharing of our uncertainties and speculations, as was appropriate for both the subject matter and the context. The workshop was organized, of necessity around the experimental work, as is this volume. Where the theoretical work is directly relevant to particular experiments, it is included in the appropriate sections with them.

Most of the participants felt strongly that magnetic fluctuations played an important role in the mechanism for high T_c, although with the exception of the μSR work reported by Luke showing results inconsistent with the anyon picture, and the work on flux phases by Lederer, the mechanism remained an issue in the background.

A major focus was the phenomenological interpretation of the NMR data. Takigawa interprets his data on ^{17}O and ^{63}Cu in terms of a single spin fluid model, supported by Rice, Bulut and Monien. Berthier argues that one needs separate degrees of freedom on the oxygen and copper to describe all the data including that from ^{89}Y. Mehring presents data on ^{205}Tl that could naturally be interpreted in terms of two fluids, points out that the two spin fluids ought to interact, and that the data could as well be described by a single spin fluid with the right fluctuation spectrum. Emery prefers to describe the situation in terms of coupled spin fluids, and Mezei cautions that even a low density of impurities may dominate the NMR relaxation in real systems.

The dramatic reduction in the NMR widths below T_c appears to require a gap opening in the fluctuation spectrum, but the neutron scattering data of Tranquada and

Shirane, and of Rossat-Mignod, clearly show spectral intensity much below any calculation of the gap energy and apparently extending to zero frequency.

There were some areas of consensus. The systematic variation of T_c with density of doped holes is demonstrated by Uemura et al. and Ansaldo, using μSR. The picture of the ground state of the Heisenberg model being Neel ordered, with well defined spin wave excitations, as in the calculations of Becher and Reiter and of Grempel, is confirmed by the neutron scattering measurements reported by Mook. The existence of quasiparticles in the t-J model is a theme in the works of Prelovsek, of Stephan and Horsch, and of Gunn, although Emery and Long point out that there are important differences with two band models.

Taken as a whole, the reader will find here an overview of the subject of the dynamics of magnetic fluctuations that we expect will be useful for anyone seeking an understanding of the physics of the high T_c materials from the perspective that these fluctuations matter for the mechanism, or that they are interesting in and of themselves.

We would like to thank the Texas Center for Superconductivity at the University of Houston, and the Mitos Corporation at the University of Crete. Their clerical and logistical support made a major contribution to the smooth working of the conference.

G. Reiter

P. Horsch

G. Psaltakis

CONTENTS

A. Neutron Scattering

B. NMR

C. μSR

D. Raman Scattering

E. Photoemission

F. Macroscopic Fluctuations

G. Transport Properties

H. General Theory

I. One Band Hubbard Models

J. Heisenberg Model Dynamics

K. Quasiparticles and Magnetic Fluctuations

ANTIFERROMAGNETIC SPIN FLUCTUATIONS IN CUPRATE SUPERCONDUCTORS

J. M. Tranquada and G. Shirane

Physics Department
Brookhaven National Laboratory
Upton, NY 11973

Introduction

In this paper we will discuss the results of some neutron scattering studies of antiferromagnetic spin fluctuations in the superconductors $YBa_2Cu_3O_{6+x}$ and $La_{2-x}Sr_xCuO_4$. We begin by discussing spin wave measurements in the antiferromagnetic phases of these compounds and comparisons between experimental and theoretical results for the spin-$\frac{1}{2}$ Heisenberg model in two dimensions. Next, recent studies of antiferromagnetic excitations in metallic and superconducting phases are described. In particular, the topics of incommensurate scattering, the temperature dependence of the spin susceptibility, and the existence of spin fluctuations at temperatures below the superconducting transition temperature will be covered. Finally, we consider the connection between neutron scattering measurements and studies of nuclear spin relaxation rates obtained by nuclear magnetic resonance. The paper concludes with a short summary.

Insulating Phases

Magnetic Order in $YBa_2Cu_3O_{6+x}$

Before discussing spin waves in antiferromagnetic $YBa_2Cu_3O_{6+x}$, it may be helpful to review the phase diagram shown in Fig. 1. (The discussion here will be kept short; further details are available elsewhere.[1–3]) At $x = 0$ the crystal exhibits a simple Néel structure involving the $Cu(2)^{2+}$ ions in the CuO_2 layers [see Fig. 2(a)]. The two-fold coordinated $Cu(1)^{1+}$ ions are nonmagnetic, and so do not participate in the magnetic structure. When oxygen is added, it goes into the Cu(1) layer converting some Cu^{1+} to Cu^{2+}(Ref. 4). Beyond $x = 0.2$, the added oxygens begin to form O–Cu(1)–O chain segments,[5] which results in a low density of O 2p holes. The Néel temperature stays constant below $x = 0.2$,[2] but begins to decrease beyond that point as a very small density of holes enters the CuO_2 planes and causes some disorder. The increased disorder is also reflected in the decrease in the average ordered moment observed at low temperature with increasing x.[2,6]

Dynamics of Magnetic Fluctuations in High-Temperature Superconductors
Edited by G. Reiter *et al.*, Plenum Press, New York, 1991

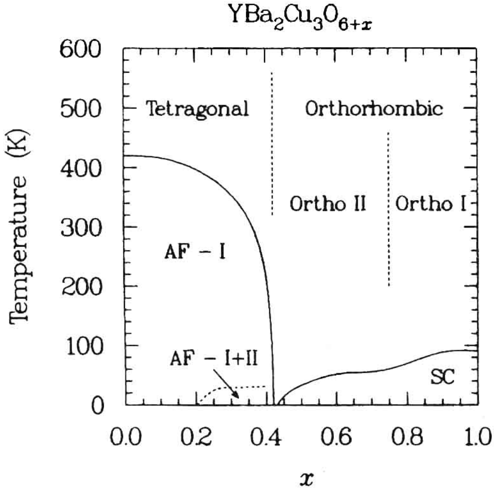

Fig. 1. Phase diagram of $YBa_2Cu_3O_{6+x}$. The positions of the phase boundaries with respect to x depend on sample preparation and treatment.

The $Cu(1)^{2+}$ ions which are formed by adding oxygen would like to couple ferromagnetically to the CuO_2 layers,[7] but they are frustrated by the antiferromagnetic coupling between the planes. Ferromagnetic coupling across the Cu(1) layer would lead to a doubling of the unit cell along the c axis, and would result in a significant hyperfine field at the Cu(1) sites. Such a magnetic structure is induced at low temperature by replacing as little as 1% of the Cu(1) sites with Fe.[8] Without doping, such long-range order does not occur.[8] A study[9] of magnetic susceptibility revealed a Curie-like contribution with an effective moment that increases with x up to $x \sim 0.3$, but which decreases sharply for temperatures below $\sim$ 30 K. Monte Carlo simulations of the magnetic lattice including some magnetic $Cu(1)^{2+}$ sites give a reasonable description of this behavior.[9] The average ordered moment measured by neutron diffraction is also observed to decrease below $\sim$ 30 K for $x \gtrsim 0.2$.[2] In a crystal with $x \approx 0.3$ we have observed excess inelastic magnetic scattering which peaks near 30 K; below this temperature diffuse elastic 2D scattering appears.[10] Rossat-Mignod *et al.*[11] have argued that the low-temperature transition is due entirely to localization of holes in the CuO_2 layers. Alternatively, we have suggested[10] that the transition involves local ferromagnetic coupling of $Cu(1)^{2+}$ ions to the planes; such defects in the magnetic order of the planes should provide good sites for holes to localize.

Spin Waves in Antiferromagnetic $YBa_2Cu_3O_{6+x}$

We have made extensive measurements[10] of spin waves in a large crystal ($\sim$ 0.5 cm^3) of $YBa_2Cu_3O_{6+x}$ with $x \approx 0.3$ and $T_N = 260$ K. Most of the measurements were made at 200 K, where little scattering is expected from $Cu(1)^{2+}$ ions. For an antiferromagnet, the long-wavelength spin-wave dispersion is given by $\omega = cq$, where c is the spin-wave velocity and q is the wave vector measured relative to a magnetic Bragg peak. The dispersion is dominated by the in-plane superexchange $J_{\parallel}$ between nearest-neigbor Cu atoms. As a result, if we hold the energy transfer ΔE $(= \hbar\omega)$ constant and scan the wave vector across the 2D rod [scan A in Fig. 2(b)], then we expect to see spin-wave peaks at $q_{\parallel} = \pm\omega/c$, where $q_{\parallel}$ is the component of the AF wave vector perpendicular to the 2D rod, and $c = \sqrt{2}J_{\parallel}a$. Examples of such scans, measured at three different excitation energies, are shown in Fig. 3. Because of the coarse spec-

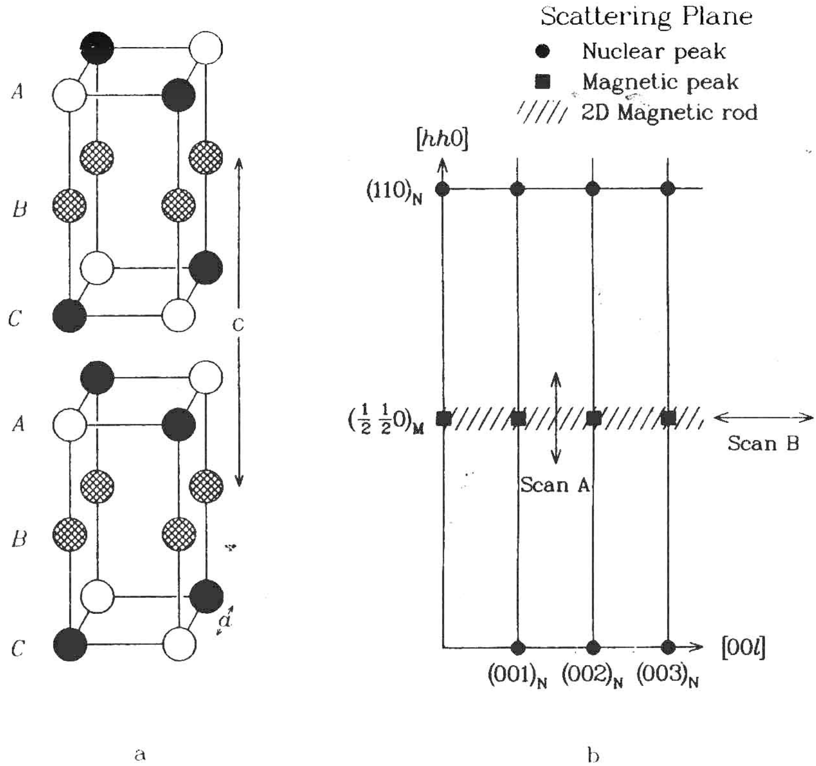

Fig. 2. (a) Magnetic spin arrangement in $YBa_2Cu_3O_{6+x}$ with x near zero. Cross-hatched circles represent nonmagnetic Cu^{1+} ions, while solid and open circles indicate antiparallel spins at Cu^{2+} sites. (b) Reciprocal space (hhl) zone. The hatched line along $(\frac{1}{2}, \frac{1}{2}, l)$ is the magnetic rod for two-dimensional scattering, and A and B indicate scans across and along the rod, respectively.

trometer resolution relative to the extremely steep dispersion, the spin-wave peaks are not resolved. The solid lines are fits made using the standard Heisenberg-model spin-wave cross section (with no damping) and taking into account the spectrometer resolution function. The amplitude was adjusted for each data set, but the overall variation was less than 10%. Equally good agreement was obtained for fits to a range of measurements, indicating that the spin waves are well described by the Heisenberg model. The value of $J_{||}$ obtained from the fits in Fig. 3, 80^{+60}_{-30} meV, is rather imprecise, but it is consistent with the somewhat larger value extracted from Raman scattering studies[12] and from higher-resolution neutron scattering measurements.[13]

For a perfectly 2D system, the spin-wave intensity should not vary significantly as the wave vector is scanned perpendicular to the planes [scan B in Fig. 2(b)]. However, as shown in Fig. 4, the spin-wave intensity measured in such a scan in $YBa_2Cu_3O_{6.3}$ is strongly modulated. There are two reasons for this modulation. The first is that because there are two CuO_2 layers per unit cell separated along the c axis by an arbitrary distance zc, the Cu atoms do not form a Bravais lattice. As a result, the spin-wave modes are split into acoustic and optical branches.[14] The second reason

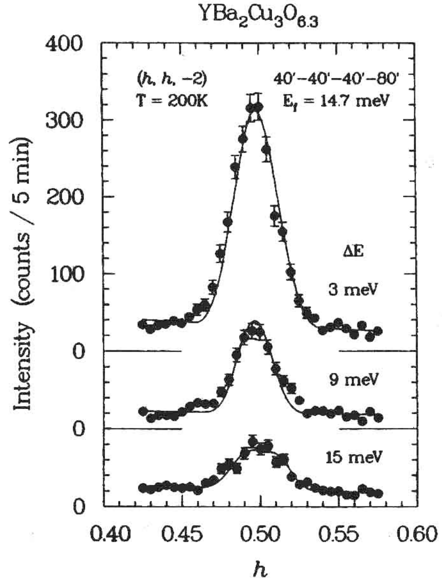

Fig. 3. Several constant ΔE scans of type A [see Fig. 2(b)] across the 2D magnetic rod in a $YBa_2Cu_3O_{6+x}$ single crystal at 200 K. The solid lines are fits to the data as discussed in the text. From Ref. 10.

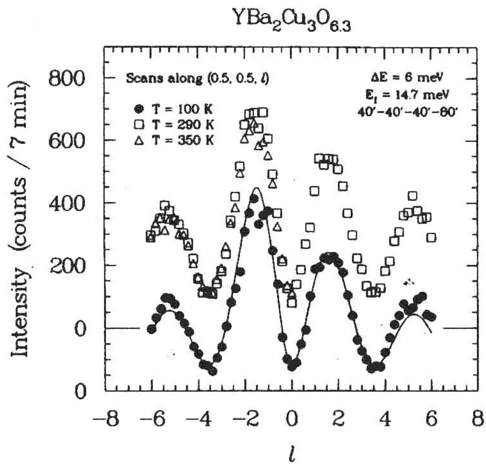

Fig. 4. Constant ΔE scan of type B [see Fig. 2(b)] along the 2D rod with $\Delta E = 6$ meV for $YBa_2Cu_3O_{6.3}$ at several temperatures. The modulation is due to the inelastic structure factor. The solid line is a fit. From Ref. 10.

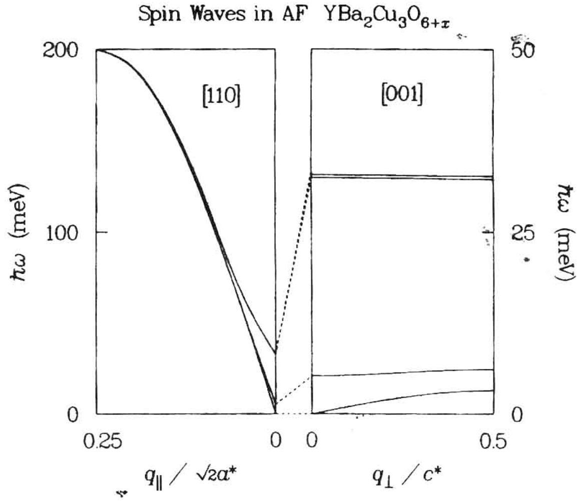

Fig. 5. Schematic diagram of spin-wave dispersion in $YBa_2Cu_3O_{6+x}$. Note that the energy scales for the two panels differ by a factor of four. The 2D nature of the magnetic interactions makes the dispersion very large along $q_{\|}$ but extremely weak along $q_{\perp}$. From Ref. 10.

is that because of a reasonably strong coupling $J_{\perp 1}$ between nearest-neighbor layers, presumably due to direct exchange along the c axis between neighboring Cu atoms, the optical modes are at energies greater than 30 meV. Assuming $J_{\|} = 80$ meV, we obtain the limit $J_{\perp 1} \gtrsim 2$ meV. Thus, at 6 meV one observes only acoustic modes modulated by the appropriate inelastic structure factor. The modulation provides a useful signature for correlations within the bilayers. In particular, it is found that the modulation survives above T_N, indicating that the bilayers remain strongly correlated in the absence of long-range order.

To complete the picture of spin-wave dispersion it is necessary to take into account the weak coupling $J_{\perp 2}$ between next-nearest-neighbor CuO_2 planes, separated by a CuO_x layer. This interaction causes a weak dispersion as a function of the wave vector component $q_{\perp}$ perpendicular to the planes. There is also a weak XY-like anisotropy of the in-plane exchange which causes a splitting of the acoustic and optical modes (each of which would otherwise be doubly degenerate). A schematic diagram of the spin-wave dispersion is shown in Fig. 5. The values of $J_{\perp 2}$ and the exchange anisotropy are on the order of $10^{-4} \times J_{\|}$. The overall picture we have obtained for spin-wave dispersion in $YBa_2Cu_3O_{6+x}$ is quite similar to that determined by Rossat-Mignod and coworkers.[11,13]

Spin Fluctuations in La_2CuO_4

Studies of the magnetic structure and spin waves in doped and undoped La_2CuO_4 have been reviewed by Birgeneau and Shirane.[15] More recently, Yamada *et al.*[16] have performed an extensive inelastic neutron scattering study on a La_2CuO_4 crystal with $T_N = 245$ K at temperatures up to 520 K. They compared their measurements with the theoretical formula for the dynamical structure factor $S(\mathbf{q}, \omega)$ determined by Chakravarty and coworkers[17,18] in their analysis of the 2D, spin-$\frac{1}{2}$ Heisenberg model. Inelastic scattering measurements above T_N were well described

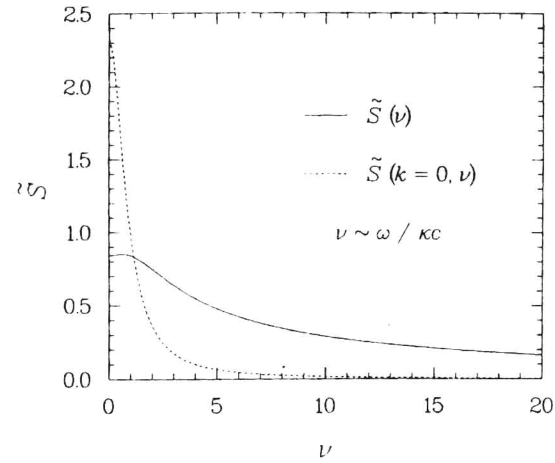

Fig. 6. The scaling function $\tilde{S}(k,\nu)$ for $k=0$, and also integrated over k, plotted vs. ν. The region of critical scattering is $\nu \lesssim 1$.

by the theoretical formula when the experimentally determined correlation length was used. The only discrepancy was an excess elastic component observed experimentally whose origin was attributed to magnetic defects. The temperature dependence of the correlation length was also in good agreement with the theoretical result.

As the correlation length ξ grows and the Néel temperature is approached from above, one expects to observe a critical slowing down of the spins. This effect should manifest itself as a sharp peak in $S(\mathbf{q},\omega)$ at $\mathbf{q}=0$ having a width $\Gamma/\hbar \approx \kappa c$, where $\kappa = 1/\xi$. For a 2D Heisenberg system, this quasielastic peak evolves into the antiferromagnetic Bragg rod at $T=0$. Because of the very strong superexchange within an insulating CuO_2 layer, ξ is several hundred anstroms even at 300 K, and correspondingly $\Gamma \sim 1$ meV.[19] Capellmann and coworkers[20] have argued that since the expected quasielastic scattering has not been directly observed in neutron scattering measurements, the picture of fixed, localized moments on the Cu atoms implicit in applications of the Heisenberg model does not properly characterize the CuO_2 layers above T_N. However, the theoretical form of $S(\mathbf{q},\omega)$ given by Tyč *et al.*[18] and tested by Yamada *et al.*[16] does contain the expected quasielastic component. Why is this component not obvious in the neutron scattering measurements?

The dynamical structure factor of Tyč *et al.*,[18] appropriate at low temperatures and frequencies, can be written as

$$S(q,\omega) = \omega_0^{-1} S_0 \tilde{S}(k,\nu), \tag{1}$$

where $\nu \equiv \omega/\omega_0$, $k \equiv q/\kappa$, and

$$\omega_0 \equiv \kappa c \sqrt{k_B T / AJ}, \tag{2}$$

with $A = 0.944$. To analyze the quasielastic component it is sufficient to consider the scaling function $\tilde{S}$. The quasielastic regime in which spin fluctuations are overdamped corresponds to $\omega < \omega_0$ (i.e. $\nu < 1$). Figure 6 shows the function $\tilde{S}(k=0,\nu)$, which clearly has most of its weight below $\nu = 1$. If the neutron scattering measurements were performed with infinite resolution, then one should indeed observe

