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Magnetic neutron scattering resonance of high- T_c superconductors in external magnetic fields: An SO(5) study

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The magnetic resonance at 41 meV observed in neutron scattering studies of $\text{YBa}_2\text{Cu}_3\text{O}_7$ holds a key position in the understanding of high- T_c superconductivity. Within the SO(5) model for superconductivity and antiferromagnetism, we have calculated the effect of an applied magnetic field on the neutron scattering cross section of the magnetic resonance. In the presence of Abrikosov vortices, the neutron scattering cross section shows clear signatures of not only the fluctuations in the superconducting order parameter ψ , but also the modulation of the phase of ψ due to vortices. In reciprocal space we find that (i) the scattering amplitude is zero at $(\pi/a, \pi/a)$, (ii) the resonance peak is split into a ring with radius π/d centered at $(\pi/a, \pi/a)$, d being the vortex lattice constant, and consequently, (iii) the splitting π/d scales with the magnetic field as \sqrt{B} .

Soon after the discovery of high- T_c superconductivity in the doped cuprate compounds, its intimate relation to antiferromagnetism was realized. A key discovery in the unraveling of this relationship was the observation of the so-called 41-meV magnetic resonance¹⁻³ later also denoted the π resonance. In inelastic neutron scattering experiments on $\text{YBa}_2\text{Cu}_3\text{O}_7$ at temperatures below $T_c \sim 90$ K, Rossat-Mignod *et al.*¹ found a sharp peak at $\hbar\omega \sim 41$ meV and $\mathbf{q} = (\pi/a, \pi/a)$, a being the lattice constant of the square lattice in the copper-oxide planes. Later its antiferromagnetic origin was confirmed by Mook *et al.*² in a polarized neutron scattering experiment and subsequently Fong *et al.*³ found that the magnetic scattering appears only in the superconducting state. Recently, Fong *et al.*⁴ have also observed the π resonance in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$, which means that it is a general feature of high- T_c superconductors and not a phenomenon restricted to $\text{YBa}_2\text{Cu}_3\text{O}_7$. This gives strong experimental evidence for the π resonance being related to antiferromagnetic fluctuations within the superconducting state. Conversely, it may be noted that angular-resolved photoemission spectroscopy has shown how the single-particle gap within the antiferromagnetic state inherits the d -wave modulation of the superconducting state.^{5,6}

A number of different models have been proposed to explain the π resonance.⁷⁻¹⁴ In particular, Zhang was inspired by the existence of antiferromagnetic fluctuations in the superconducting state to suggest a unified SO(5) theory of antiferromagnetism and d -wave superconductivity in the high- T_c superconductors.¹⁰ It is of great interest to extend the different theoretical explanations to make predictions for the behavior of the π resonance, e.g., in an applied magnetic field. An experimental test of such predictions will put important constraints on theoretical explanations of the π resonance in particular and of high- T_c superconductivity in general. In this paper we treat the π resonance in the presence of an applied magnetic field within the SO(5) model.

Zhang proposed that the cuprates at low temperatures can be understood as a competition between d -wave supercon-

ductivity and antiferromagnetism of a system which at higher temperatures possesses SO(5) symmetry.¹⁰ The SO(5) symmetry group is the minimal group that contains both the gauge group U(1) [=SO(2)] which is broken in the superconducting state, and the spin rotation group SO(3) which is broken in the antiferromagnetic state. Furthermore, the SO(5) group also contains rotations of the superspin between the antiferromagnetic sector and the superconducting sector. The relevant order parameter is a real vector $\mathbf{n} = (n_1, n_2, n_3, n_4, n_5)$ in a five-dimensional superspin space with a length which is fixed ($|\mathbf{n}|^2 = 1$) at low temperatures. This order parameter is related to the complex superconducting order parameter ψ and the antiferromagnetic order parameter \mathbf{m} in each copper-oxide plane as follows: $\psi = fe^{i\phi} = n_1 + in_5$ and $\mathbf{m} = (n_2, n_3, n_4)$. Zhang argued how in terms of the five-dimensional superspin space one can construct an effective Lagrangian $\mathcal{L}(\mathbf{n})$ describing the low-energy physics of the t - J limit of the Hubbard model.

Two comments are appropriate here. First, we note that relaxing the constraint $|\mathbf{n}|^2 = 1$ in the bulk superconducting state will introduce high energy modes, but these can safely be ignored at low temperatures. Moreover, they do not alter the topology of vortices in the order parameter, which is our main concern. Second, one may worry that results obtained from a pure SO(5) model deviate substantially from those obtained from the recently developed, physically more correct projected SO(5) theory.¹⁵ However, the two models are only significantly different close to half filling, and our study concerns antiferromagnetic (AF)-modes in the bulk superconductor in a weak magnetic field, a state which although endowed with the topology of vortices is far from half filling. For simplicity, we thus restrict the calculations in this paper to the original form of the SO(5) theory.

In the superconducting state the SO(5) symmetry is spontaneously broken which leads to a ‘‘high’’-energy collective mode where the approximate SO(5) symmetry allows for rotations of \mathbf{n} between the superconducting and the antiferromagnetic phases. These rotations have an energy cost $\hbar\omega_\pi$ corresponding to the π resonance and fluctuations in \mathbf{n} will thus give rise to a neutron scattering peak at $\hbar\omega_\pi$ which,

through the antiferromagnetic part of the superspin, is located at $\mathbf{q}=\mathbf{Q}$, where $\mathbf{Q}=(\pi/a,\pi/a)$ is the antiferromagnetic ordering vector. The uniform superconducting state ($f=1$) can be characterized by a superspin $\mathbf{n}=(f\cos\phi,0,0,f\sin\phi)$, and the π mode is a fluctuation $\delta\mathbf{n}(t)\propto(0,0,0,f e^{i\omega\pi t},0)$ around the static solution, where $\hat{\mathbf{z}}$ has been chosen as an arbitrary direction for $\delta\mathbf{m}$. In this case with $f=1$ we have $\delta\mathbf{m}\propto e^{i\omega\pi t}$, i.e., a sharp peak at $\omega=\omega_\pi$ and $\mathbf{q}=\mathbf{Q}$.

In the presence of an applied magnetic field, the superconductor will be penetrated by flux quanta, each forming a vortex with a flux $h/2e$ by which the complex superconducting order parameter ψ acquires a phase shift of 2π when moving around the vortex. In $\text{YBa}_2\text{Cu}_3\text{O}_7$ the vortices arrange themselves in a triangular vortex lattice¹⁶ with an area of the hexagonal unit cell given by $\mathcal{A}=h/2eB$ and consequently a lattice constant given by $d=3^{-1/4}\sqrt{h/eB}$. In the work by Arovas *et al.*,¹⁷ Bruus *et al.*,¹⁸ and Alama *et al.*¹⁹ the problem of Abrikosov vortices was studied within the SO(5) model of Zhang.¹⁰ In the center of a vortex core, the superconducting part of the order parameter is forced to zero. This leaves two possibilities: (i) either the vortex core is in a metallic normal state (as it is the case in conventional superconductors) corresponding to a vanishing superspin or (ii) the superspin remains intact but is rotated from the superconducting sector into the antiferromagnetic sector.¹⁷ The prediction of the possibility of antiferromagnetically ordered insulating vortex cores is thus quite interesting and allows for a direct experimental test of the SO(5) theory. However, the antiferromagnetic ordering of vortices is according to our knowledge still to be confirmed experimentally. In this paper we report a different consequence of the SO(5) theory in neutron scattering experiments; we consider the π mode in the presence of vortices and show that the peak at $\mathbf{q}=\mathbf{Q}$ splits into a ring with a radius π/d centered at $\mathbf{q}=\mathbf{Q}$ where it has zero amplitude. Consequently the splitting scales with magnetic field B as $\pi/d\propto\sqrt{B}$.

We start by considering just one vortex, then generalize the result to a vortex lattice. To make our calculations quantitative, we consider $\text{YBa}_2\text{Cu}_3\text{O}_7$ for which $a=3.8\text{ \AA}$, $\kappa\simeq 84$, and $\xi\simeq 16\text{ \AA}$ for the lattice constant, the Ginzburg-Landau parameter, and the coherence length, respectively. The order parameter can be written in the form¹⁸

$$\mathbf{n}(\mathbf{r})=(f(r)\cos\phi_r,0,m(r),0,f(r)\sin\phi_r), \quad (1)$$

where $\phi_r=\arg(\mathbf{r})$. The isotropy of the antiferromagnetic subspace allows us to choose \mathbf{m} to lie in the y direction without loss of generality. Static numerical solutions for $f(r)$ and thereby also $m(r)$ in the presence of a vortex are derived as described in Refs. 17 and 18. Due to the high value of κ the absolute value f of the superconducting order parameter ψ increases from zero at the center of the vortex ($r=0$) to its bulk value ($f=1$) at a distance of the order ξ from the center. The antiferromagnetic order parameter follows from f since $m=\sqrt{1-f^2}$.

For the π mode in the presence of a vortex, Bruus *et al.*¹⁸ found that the fluctuation of the superspin is

$$\delta\mathbf{n}(\mathbf{r},t)=(0,0,0,\delta\theta f(r)\cos\phi_r e^{i\omega\pi t},0), \quad (2)$$

where the small angle $\delta\theta$ by which \mathbf{n} rotates into the antiferromagnetic sector is undetermined. Since the excitation depends on f and not on m it is a delocalized excitation with zero amplitude at the center of the vortices and in terms of energy it actually corresponds to an energy at the bottom edge of the continuum of an effective potential associated to the vortices.¹⁸

For an isotropic spin space, the magnetic scattering cross section for neutrons is proportional to the dynamic structure factor, which is the Fourier transform of the spin-spin correlation function (see, e.g., Ref. 20),

$$\mathcal{S}(\mathbf{q},\omega)=\int_{-\infty}^{\infty} dt e^{i\omega t} \sum_{\mathbf{R},\mathbf{R}'} e^{-i\mathbf{q}\cdot(\mathbf{R}-\mathbf{R}')} \langle \hat{\mathbf{S}}_{\mathbf{R}}(t) \cdot \hat{\mathbf{S}}_{\mathbf{R}'}(0) \rangle. \quad (3)$$

To make a connection to the SO(5) calculations we make the semiclassical approximation $\langle \hat{\mathbf{S}}_{\mathbf{R}}(t) \cdot \hat{\mathbf{S}}_{\mathbf{R}'}(0) \rangle \approx \langle \hat{\mathbf{S}}_{\mathbf{R}}(t) \rangle \cdot \langle \hat{\mathbf{S}}_{\mathbf{R}'}(0) \rangle$ so that

$$\mathcal{S}(\mathbf{q},\omega) \approx \int_{-\infty}^{\infty} dt e^{i\omega t} \sum_{\mathbf{R},\mathbf{R}'} e^{-i(\mathbf{q}+\mathbf{Q})\cdot(\mathbf{R}-\mathbf{R}')} \mathbf{m}(\mathbf{R},t) \cdot \mathbf{m}(\mathbf{R}',0), \quad (4)$$

where $\mathbf{m}(\mathbf{R},t)=e^{i\mathbf{Q}\cdot\mathbf{R}}\mathbf{S}_{\mathbf{R}}(t)$ is the antiferromagnetic order parameter which enters the superspin \mathbf{n} .

With a superspin given by $\mathbf{n}(\mathbf{r},t)=\mathbf{n}(\mathbf{r})+\delta\mathbf{n}(\mathbf{r},t)$ the dynamical structure factor has two components—an elastic and an inelastic. The elastic component,

$$\mathcal{S}_{\text{el}}(\mathbf{q},\omega)=\left| \sum_{\mathbf{R}} e^{-i(\mathbf{q}+\mathbf{Q})\cdot\mathbf{R}} m(\mathbf{R}) \right|^2 2\pi\delta(\omega), \quad (5)$$

is located at $\mathbf{q}=\mathbf{Q}$ and has a width $\sim\pi/\xi$. In elastic neutron scattering experiments the observation of this peak would directly prove the antiferromagnetic ordering in vortex cores.

The inelastic contribution is

$$\mathcal{S}_{\text{in}}(\mathbf{q},\omega)=(\delta\theta)^2 \left| \sum_{\mathbf{R}} e^{-i(\mathbf{q}+\mathbf{Q})\cdot\mathbf{R}} f(R) \cos\phi_{\mathbf{R}} \right|^2 2\pi\delta(\omega-\omega_\pi). \quad (6)$$

For $\mathbf{q}=\mathbf{Q}$ the phase factor $e^{-i(\mathbf{q}+\mathbf{Q})\cdot\mathbf{R}}$ vanishes, and the cosine factor makes the different terms in the summation cancel pairwise so that $\mathcal{S}_{\text{in}}(\mathbf{Q},\omega_\pi)=0$. The presence of a single vortex moves the intensity away from $\mathbf{q}=\mathbf{Q}$ and a ring-shaped peak with radius $\delta q\sim\pi/L$ centered at $\mathbf{q}=\mathbf{Q}$ is formed, $L\sim\sqrt{A}$ being the size of the sample. In the semiclassical approximation the zero amplitude at $\mathbf{q}=\mathbf{Q}$ is a topological feature, which is independent of the detailed radial form $f(r)$ of the vortex. This robustness relies on the identification of the π mode as being proportional to the superconducting order parameter (including its phase). Quantum fluctuations may add some amplitude at $\mathbf{q}=\mathbf{Q}$, but such an analysis beyond leading order is outside the scope of this work.

It is interesting to see how this result compares to predictions based on the BCS theory. The neutron scattering cross section is given by the spin susceptibility, which for a homogeneous (vortex free) superconductor has been calculated via the BCS-Lindhard function.^{8,9} Here we briefly consider how the BCS coherence factor $[u_k v_{k+q} - v_k u_{k+q}]^2$ appearing in

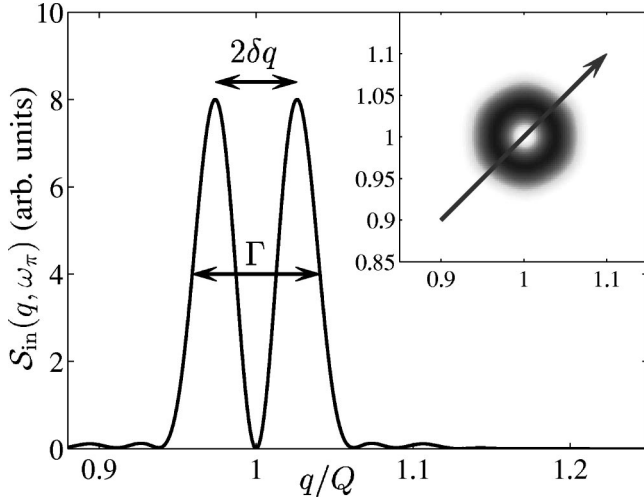


FIG. 1. Plot of the dynamic structure factor at $\omega = \omega_\pi$ as a function of q along the (π, π) direction for $B=10$ T. The inset shows the almost isotropic response in the q plane with the arrow indicating the (π, π) direction.

the Lindhard function²¹ is modified by the presence of vortices. In a semiclassical approximation²² the spatial variation of the superconducting phase $\phi(\mathbf{r})$ leads to a coherence factor of the form $[u_k(\mathbf{r}_1)e^{i\phi(\mathbf{r}_1)/2}v_{k+q}(\mathbf{r}_2)e^{i\phi(\mathbf{r}_2)/2} - v_k(\mathbf{r}_1)e^{i\phi(\mathbf{r}_1)/2}u_{k+q}(\mathbf{r}_2)e^{i\phi(\mathbf{r}_2)/2}]^2$. Therefore in contrast to Eq. (6) the superconducting phase does not separate in the two spatial positions, and consequently the spatial average in general is not zero at $\mathbf{q}=\mathbf{Q}$. It thus appears that the above-mentioned ring-shaped peak in the dynamic structure factor is special for the SO(5) model.

We now generalize the single-vortex SO(5) result to the case of a vortex lattice. For nonoverlapping vortices we construct the full superconducting order parameter by

$$\tilde{\psi}(\mathbf{r}) = \tilde{f}(\mathbf{r})e^{i\tilde{\phi}(\mathbf{r})} = \prod_j \psi(\mathbf{r} - \mathbf{r}_j), \quad (7)$$

where the \mathbf{r}_j denote the positions of the vortices. The function $\tilde{f}(\mathbf{r}) = \prod_j f(\mathbf{r} - \mathbf{r}_j)$ is 1 except for close to the vortices where it dips to zero. Also the phase $\tilde{\phi}(\mathbf{r}) = \sum_j \arg(\mathbf{r} - \mathbf{r}_j)$ has by construction the periodicity of the vortex lattice (modulo 2π) and the contour integral $\oint_C d\mathbf{l} \cdot \nabla \tilde{\phi}(\mathbf{r})$ equals $2\pi n$ where n is the number of vortices enclosed by the contour C . In the limit of nonoverlapping vortices we can capture the main physics by considering the single vortex solution within a unit cell of the vortex lattice. We comment on the inclusion of the entire vortex lattice further on, but for now we restrict the summation in Eq. (6) to lattice sites \mathbf{R} inside the vortex lattice unit cell. In Fig. 1 we show the result for a magnetic field $B=10$ T. As seen, the presence of vortices moves the intensity away from $\mathbf{q}=\mathbf{Q}$ and a ring shaped peak with radius δq centered at $\mathbf{q}=\mathbf{Q}$ is formed. We note that the only relevant length scale available is the vortex lattice constant d and consequently we expect that $\delta q = \pi/d$. Since $d = 3^{-1/4} \sqrt{\hbar/eB}$ we consequently expect that $\delta q = 3^{1/4} \pi \sqrt{eB/\hbar} \approx 0.008 \times (\pi/a) \sqrt{B/[T]}$. Had we included all the vortex lattice unit cells in our analysis, the structure factor of the hexagonal vortex lattice would have led to a breaking of the ring in Fig. 1 into six subpeaks sitting on top of the

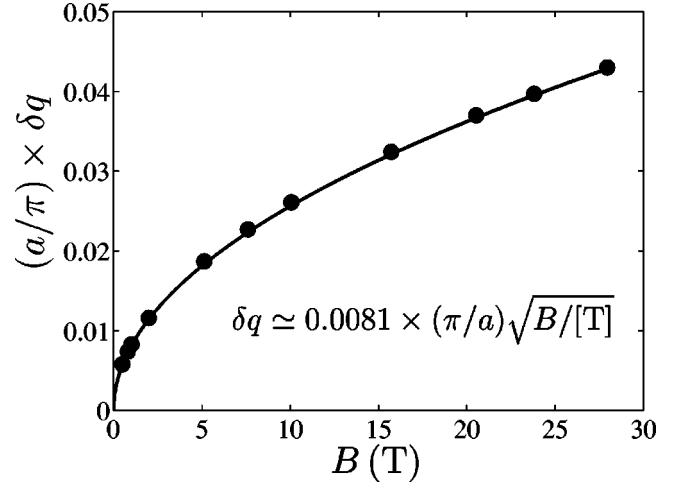


FIG. 2. Plot of the peak splitting δq as a function of the magnetic field B . The calculated splitting (\bullet) has the expected $B^{1/2}$ behavior and the numerical prefactor corresponds to a splitting $\delta q = \pi/d$ where d is the vortex distance.

ring. In a real experiment these subpeaks could easily be smeared back into a ring-shaped scattering peak if either the vortex lattice were slightly imperfect or if the resolution of the spectrometer were too low. To describe the main effect of the SO(5) theory we therefore continue to use the single unit-cell approximation.

In Fig. 2 we show the splitting as a function of the magnetic field and indeed we find the expected scaling with a prefactor confirming that the splitting is given by $\delta q = \pi/d$. The full width half maximum of the ring is given by $\Gamma \approx 3.1 \times \delta q = 3.1 \times \pi/d$.

In Fig. 3 we show the amplitude of the ring as a function of magnetic field. The amplitude approximately decreases as $1/B$ with the magnetic field, but with a small deviation. This deviation makes the \mathbf{q} -integrated intensity, which is proportional to the amplitude times $(\delta q)^2$, decrease as $I(B)/I(0) \approx 1 - 0.004 \times B/[T]$ which reflects that the area occupied by vortices increases linearly with B and consequently the superconducting region decreases linearly with B . In fact, the reduction is given by $\mathcal{A}^{-1} 2\pi \int r dr m^2(r) \approx 0.004 \times B/[T]$,

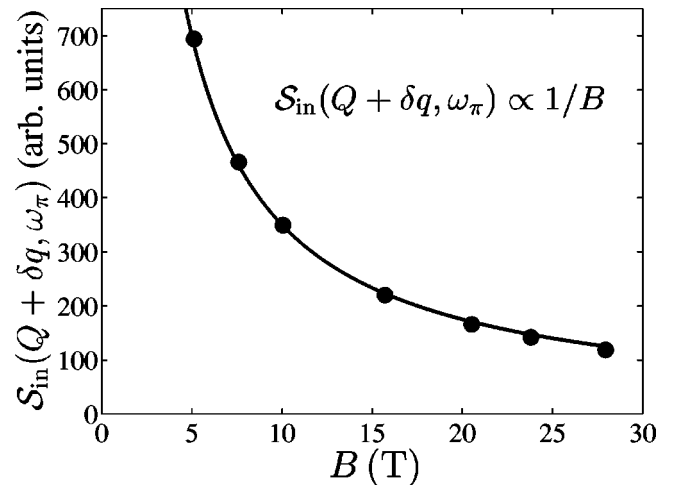


FIG. 3. The peak height plotted versus the magnetic field B . The calculations (\bullet) almost fit a $1/B$ dependence.

where the integral gives the effective area of the vortex. The reduction in integrated intensity should be relatively easy to observe experimentally, but is not a unique feature of the SO(5) model. Thus while it will aid us to prove that the π resonance only resides in the superconducting phase, it will not clearly distinguish between different theories.

In order to discuss the experimental possibilities for testing our predictions, we note that the original observation of the zero-field π resonance was an experimental achievement and hence that the experiment proposed here constitutes a great challenge. However, since the observation of the π resonance in 1991, the field of neutron scattering has developed considerably. To observe the ringlike shape (see inset of Fig. 1) of the excitation would require a resolution better than π/d along two directions in reciprocal space, which seems unachievable with current spectrometers. However, the overall width of the ring can in fact be measured with good resolution along just one direction in the reciprocal plane. Scans along this direction (as in Fig. 1) could then reveal a broadening of $\sim 3.1 \times \pi/d$. With a sufficiently opti-

mized spectrometer we believe this to be possible, and the reward is a stringent test of a quantitative prediction of the SO(5) theory. We note that Bourges *et al.*²³ have investigated the π resonance in a magnetic field of $B = 11.5$ T and report a broadening in energy, but do not report data on the \mathbf{q} shape.

In conclusion, we have found that within the SO(5) model, the π resonance splits into a ring centered at $\mathbf{q} = (\pi/a, \pi/a)$ in the presence of a magnetic field. The ring has the radius π/d and full width half maximum of about $3.1 \times \pi/d$, where d is the vortex lattice constant. Consequently the splitting is found to scale with the magnetic field as $B^{1/2}$. We emphasize that the amplitude of the π resonance is zero at $\mathbf{q} = (\pi/a, \pi/a)$ in the presence of a magnetic field.

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