Theory of the hourglass dispersion of magnetic excitations in high-$T_c$ cuprates

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Abstract – A theory for the dispersion of collective magnetic excitations in superconducting cuprates is presented with the aim to cover both high- and low-doping regimes. Besides of spin fluctuations describable in the random phase approximation (RPA) we allow for local spin rotations within a mode-coupling theory. At low temperatures and moderately large correlation lengths we obtain two branches of excitations which disperse up- and downwards exhibiting the hourglass behavior observed experimentally at intermediate dopings. At large and small dopings our theory essentially reduces to the RPA and spin wave theory, respectively.

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The low-temperature magnetic response of many high-$T_c$ superconductors such as YBCO [1,2] and Bi2212 [3,4] is characterized by a resonant mode inside the superconducting gap around the antiferromagnetic wave vector $Q$. This collective mode manifests itself as a single peak at $Q$ which splits into two peaks dispersing up- and downwards in frequency away from $Q$. This unusual dispersion resembles the shape of a hourglass. A similar dispersion has been observed also in 214 cuprates [5,6]. Several theories to explain this phenomena are based on static or dynamic stripes neglecting superconductivity [7–10]. Such an approach seems to be most suitable for 214 cuprates where stripes have been detected and used to explain various properties of these systems [5]. Other theories disregard stripes but include superconductivity and use a rather local [11,12] or an itinerant [13–16] description for the magnetism. These theories should be applicable to YBCO and Bi2212 because the resonance mode in these systems is roughly proportional to $T_c$ and thus closely tight to superconductivity. The simplest itinerant theory for the resonant mode and its dispersion considers particle-hole excitations with spin-flips interacting within the random phase approximation (RPA) forming a dispersing bound state in the superconducting gap.

In the following we present a theory which overcomes some of the shortcomings of the RPA approach. The latter yields only one branch of excitations below the Stoner continuum whereas it has been established recently that the lower branch, the center of the hourglass as well as part of the upper branch lie below this continuum in the gapped region [3]. A more theoretical argument for the incompleteness of a RPA description comes from the fact that the spin susceptibility is described in this approximation diagramatically by spin bubbles connected via the Heisenberg interaction. A given spin direction, for instance the $z$-direction, is conserved along the bubbles which means that the transverse part of the Heisenberg interaction, which would mix different directions, does not enter at all. The RPA thus excludes local rotations of spins which are characteristic for spin wave theory and which should play an increasing role at decreasing doping. The theory presented below contains both spin wave theory and RPA as special cases. At intermediate dopings we will show that both RPA and spin-wave-like spin fluctuations are important and produce the two branches of the hourglass dispersion.

We consider the $t$-$J$ model [17] on a square lattice with the Hamiltonian

$$H = \sum_{k\sigma} \epsilon(k) \tilde{c}_{k\sigma}^\dagger \tilde{c}_{k\sigma} + \frac{1}{2} \sum_k J(k) S_k S_{-k}. \quad (1)$$

$\tilde{c}_{k\sigma}^\dagger, \tilde{c}_{k\sigma}$ are constrained creation and annihilation operators, respectively, for electrons with momentum $k$ and spin.
projection σ excluding any double occupancies of sites. S_k
are spin operators in momentum space and ε(k) is the bare
electron dispersion given by

\[ ε(k) = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y, \]

where \( t \) and \( t' \) are hopping amplitudes between nearest and second-nearest neighbors, respectively, and the lattice constant has been put to 1. \( J(k) \) is the Fourier transform of the Heisenberg coupling between nearest neighbors. In a mean-field approximation, used in the following, the constrained operators are replaced by usual ones and the constraint is approximately taken into account by a renormalization of \( ε(k) \), for instance, by \( t \rightarrow δt \) and \( t' \rightarrow δt' \), where \( δ \) is the doping away from half-filling. Compared to the experiment this approximation yields a band which is too small at optimal doping and also depends much too strong on \( δ \) below optimal doping (see, for instance, Table I of ref. [18]). We therefore will use in the calculations eq. (2) with the experimental values for the renormalized hopping amplitudes.

In the following we are interested in the time evolution of the spin operator \( S_k \),

\[ \mathbf{A}(k,q) = \sum_{α,β} c_κ^α q_κ q_σ \sigma_{αβ} c_κ^β, \]

where \( \sigma \) denotes the vector of the three Pauli matrices. It obeys the equation of motion

\[ \frac{∂ \mathbf{A}}{∂t} = i(\mathcal{L}_0 + \mathcal{L}_1) \mathbf{A}, \]

with

\[ \mathcal{L}_0 \mathbf{A}(k,q) = (ε(k + q) - ε(q)) \mathbf{A}(k,q) + J(k)(f(k) - f(k + q)) \mathbf{S}_k, \]

\[ \mathcal{L}_1 \mathbf{A}(k,q) = \frac{1}{4} \sum_{k'} J(k') \]

\[ \cdot (\mathbf{S}_{k'} × \mathbf{A}_+(k,q) - \mathbf{A}_+(k,q) × \mathbf{S}_{k'}), \]

where \( \mathbf{A}_+(k,q) = \mathbf{A}(k - k',q) + \mathbf{A}(k - k',q') + \mathbf{A}(k',q) + \mathbf{A}(k',q'). \) \( f(k) \) is equal to \( \langle c_κ^α c_κ^β \rangle \), where \( \langle \cdots \rangle \) denotes the thermodynamic expectation value, and \( × \) stands for the vector product. Since we are only interested in the spin response we have dropped terms on the right-hand side of eq. (6) which involve fluctuations in the density. We also dropped an overall prefactor denoting the number of primitive cells. The unperturbed Liouville operator \( \mathcal{L}_0 \) describes the time evolution of the system in the RPA. From its explicit expression in eq. (5) follows that it does not mix different Cartesian components of the spin operators. In contrast to that the time evolution described by \( \mathcal{L}_1 \) involves product states of spin operators, mixes different spin components and thus can describe rotations of spins due to fluctuating fields.

The spin susceptibility \( χ(k,z) \) can conveniently be calculated from the associated Kubo relaxation function \( Φ(k,z) = (χ(k) - χ(k,z))/z \), where \( z \) is a complex frequency and \( χ(k) \) is equal to \( χ(k,z = 0) \). Due to the rotational invariance in spin space we may assume that \( χ, M \) etc. always refer to the \( z \)-direction. Using the Mori formalism \( Φ \) can be written as \[ 19] \]

\[ Φ(k,z) = \frac{χ(k)}{z + M^{RPA}(k,z) + M(k,z)}, \]

The first memory kernel \( M^{RPA}(k,z) \) describes the time evolution of spin operators by \( \mathcal{L}_0 \). It thus can be evaluated in the RPA yielding

\[ M^{RPA}(k,z) = z χ^{RPA}(k,z)/((χ^{RPA}(k) - χ^{RPA}(k,z))). \]

(8) \( χ^{RPA}(k,z) \) is the spin susceptibility in the RPA using also BCS mean-field theory to implement superconducting pairing. Strictly speaking, the right-hand side of eq. (8) contains the additional factor \( χ^{RPA}(k)/χ(k) \), which would change our results only in an unessential way and thus is neglected in the following. Inserting eq. (8) into eq. (7) and putting \( M = 0 \), \( χ(k) = χ^{RPA}(k) \) one easily verifies that the correct RPA expression for \( χ(k,z) \) is reproduced.

The leading contribution to \( M \) is obtained in second order in \( \mathcal{L}_1 \). It describes the evolution of a single spin fluctuation into product states of spin fluctuations both evolving in time with \( L_0 \) in our lowest-order approximation. Performing the analytic continuation \( z \rightarrow ω + iη \), we obtain for the imaginary part of \( M \), denoted by \( M'' \),

\[ M''(k,ω) = \sum_{k'} (J(k') - J(k - k'))^2 D''(k,k',ω)/ωχ(k), \]

(9)

\[ D''(k,k',ω) = \pi \int dw'A(k - k',ω - w)A(k',ω') \]

\[ ×(b(ω') - b(ω') - w)). \]

A is the spectral function of the spin propagator and \( b(ω') \) the Bose function.

One peculiar feature of the Mori formalism is that the static and dynamic parts of correlations functions can be considered to be independent of each other. This means that the static susceptibility \( χ(k,z = 0) \) is always equal to \( χ(k) \) independent of what approximations are made for \( M \). On the other hand \( χ(k) \) itself is not determined by eqs. (7)–(10) but must be obtained by other means. In our case we will argue that at larger dopings the RPA expression can be used for \( χ(k) \), whereas at low dopings we will parametrize \( χ(k) \) in terms of the correlation length.

Though there is no simple relation between approximations in the Mori formalism and diagrams of conventional many-body perturbation theory the following can be said in our case assuming a paramagnetic ground state. For \( M = 0 \) eq. (7) reproduces the RPA expression for \( χ(k,z) \) which is equivalent to a sum of spin bubbles connected
by the Heisenberg interaction. The memory kernel $M$ in eq. (7) represents a self-energy for the spin propagator where according to eq. (6) a spin wave polarized in the $z$-direction decays into a product state of two spin waves polarized in the $x$ and $y$ directions. Such processes correspond to diagrams where two electron propagators in two different bubbles in the RPA sum are scattered via the Heisenberg interaction and these additional Heisenberg interaction lines are joined by an arbitrary number of bubbles. To describe the undoped case correctly, one would have to include also vertex corrections in the bubbles because otherwise the bubbles are proportional to $\delta$ and thus would vanish if the constraint is strictly enforced.

**Small correlation lengths.** – In the case of small antiferromagnetic correlation lengths $\xi$, corresponding to the overdoped regime, the RPA should be a reasonable approximation for the spin susceptibility. The dashed line in fig. 1 shows the imaginary part of $\chi''(Q, \omega)$ for $Q = (\pi, \pi)$ using the parameters from table I of ref. [13] and a chemical potential corresponding to the doping $\delta = 0.2$. The energy unit is 1 eV in the following and we have included also the third- and higher-order hoppings listed in the table. The superconducting order parameter is $\Delta(k) = \Delta(\cos k_x - \cos k_y)/2$ with $\Delta = 0.029$, $J$ equal to 0.135 and $\eta = 0.004$. The dashed line in fig. 1 illustrates that most of the spectral weight resides in the bound state at the energy 0.038 and that only a small part of it has been left in the continuum at higher energies. Away from $Q$ the dashed curve in fig. 1 does not change dramatically as long as the bound state lies still in the gapped region. Entering the particle-hole continuum by going further away from $Q$ destroys the bound state and most of the spectral weight shifts to high energies of the order of $t$. The parameters used in fig. 1 yield $\xi \sim 0.78$. For such a small $\xi$ practically all momenta in the sum over momenta in eq. (9) contribute substantially which means that $M''$ is mainly determined by contributions away from the small region around $Q$ so that the bound state and its low-energy scale is rather irrelevant for $M''$.

This is confirmed by an explicit calculation of $M$ using RPA results for the various quantities in eq. (9). The result is shown in the inset of fig. 1 for $T = 0$. $M''$ (solid line) is structureless except at small energies where it vanishes rapidly due to the smallness of $A$ in this region and the cutoff $\omega$ for the integration over $\omega$ in eq. (10) due to the bosonic factors. Taking $M$ into account in eq. (7) yields the solid line in fig. 1 which differs only marginally from the dashed line. This shows that at short correlation lengths the RPA result for $\chi''$ is essentially correct and that the correction $M$ to $M^{RPA}$ is rather small. The underlying physical picture is that the momentary local axis of preferred spin directions fluctuates very rapidly due to the random forces induced by $L_4$. The spectrum of these forces is given by $M''$ and characterized by the large energy scale $t$ in agreement with the inset of fig. 1.

**Large correlation lengths.** – For large $\xi$ the spectral function $A(k, \omega)$ is strongly peaked at $k' = k$. This means that the integration over $k'$ in eq. (9) is restricted to momenta near $0$ or near $Q$. Since we are interested in external momenta $k \sim Q$ the momentum of one of the two spectral functions in eq. (10) is small. Due to spin conservation this spectral function describes spin diffusion and is mainly restricted to small values of $\omega'$. As a result one may neglect the small frequency transfer in the second spectral function in eq. (10). Taking also the real part of $M$ into account we obtain from eqs. (9) and (10),

$$M(k, \omega) = -\omega^2(k)\Phi(Q, \omega)/\chi(Q),$$

with

$$\omega^2(k) = \frac{2}{\chi(k)} \sum_q (J(q) - J(k - q))^2 \langle S_{k-q}S_{q-k} \rangle \chi(q),$$

and the equal-time correlation function

$$\langle S_k S_{-k} \rangle = \int d\omega \Phi(\omega) A(k, \omega).$$

In deriving eq. (11) we used the fact that the two memory functions in eq. (7) depend for our parameters only slowly on momentum around the wave vector $Q$ so that the combination $\Phi/\chi$ on the right-hand side of eq. (11) may be evaluated at $Q$. The sum over $q$ in eq. (12) runs over half of the Brillouin zone centered around $Q$. In the optimal and moderately underdoped region the RPA yields values for $\xi$ of one or smaller (we get for $\delta = 0.12$ $\xi \sim 0.8$, ref. [15] obtains $\xi \sim 0.6$) whereas the experimental values for $\xi$ are larger by about a factor 5 or more [20]. Since such a large discrepancy would affect severely the momentum sum in eq. (12) we will use the empirical expression $\chi(k) = \chi(Q)/(1 + \xi^2(\Delta k)^2)$ with $\Delta k = k - Q$ for the static susceptibility considering $\xi$ as a parameter to be determined from experiment.

It is instructive to study the frequency dependence of the denominator of eq. (7). In order to describe a slightly
undoped case we choose the same parameters as in fig. 1, a chemical potential corresponding to $\delta = 0.12$, $\xi = 4$, and the cutoff $1/\xi$ for the sum over $q$ in eq. (12). The solid and dotted lines in fig. 2 show $1 + M^{\text{RPA}}(k, \omega)/\omega$ for $H = 0.45$ and $0.38$, respectively, writing $k = (H, 0.45)/2\pi$. This quantity is practically independent of momentum, increases monotonically with $\omega$ and is zero at the RPA resonance energy $\omega_R \approx 0.038$. The dashed-dotted and dashed lines in fig. 2 show $-M'(k, \omega)/\omega$ for the same momenta. These curves resemble the real part of an oscillator located at $\omega_R$ with an oscillator strength being very small at $\Delta k = 0$ and strongly increasing with $|\Delta k|$. The poles of eq. (7) are given by the common points of the two curves denoted by squares and circles. Since the common point at $\omega = \omega_R$ (not shown in fig. 2) has vanishing pole strength there are only two branches of collective spin excitations. For vanishing damping $\eta$ there is shown in fig. 3 by solid lines. They nearly touch each other at $\Delta k = 0$ and disperse up- and downwards with increasing $|\Delta k|$. For not too large $|\Delta k|$ both branches lie below the continuum in agreement with experiment [3]. Performing the calculation in the normal state at $T = T_c$ the solid and dotted lines in fig. 2 lie everywhere above zero but the solid and dashed and also the dotted and dash-dotted lines have still one common point at low frequencies. In this case only the upper branch exists in agreement with experiment [2,4]. At very low dopings $M^{\text{RPA}} \to 0$ due to the constraint and the pole condition $\omega + M'(k, \omega)$ yields in the presence of long-range order the correct spin wave dispersion [19].

Several prerequisites are necessary to obtain a hourglass dispersion for spin excitations. There must exist two different kinds of spin excitations to account for the two branches. The first one are RPA spin fluctuations where all induced spin moments have the same direction. They may be characterized by the fact that the internal fields induced by the Heisenberg interaction conserves frequency, momentum and spin direction which is a direct consequence of the one-mode behavior of $\mathcal{L}_0$ in eq. (5). The second one are local rotations of spins under the influence of $\mathcal{L}_1$ in eq. (6). In this case a spin in the $z$-direction acquires in its time evolution also a component in the $x$-direction due to the presence of a spin fluctuation in the $y$-direction. The pure form of the two kind of spin excitations are obtained for $M = 0$ and $M^{\text{RPA}} = 0$, respectively, and are realized approximately at large and small dopings. In the hourglass regime $M$ and $M^{\text{RPA}}$ are of similar magnitude.

Another prerequisite for hourglass behavior is that $\xi$ is substantially larger than 1. Only then is the momentum integration in eq. (9) restricted to the resonance and the spin diffusion mode, yielding oscillator-like behavior of $M$ near $\omega_R$. The up- and downwards dispersion and their approximate degeneracy at $Q$ is mainly determined by $\omega^2(k)$, which according to eq. (12) is roughly proportional to $(S(k)S(-k))^{-1/2}(\xi^2 + (\Delta k)^2)$. The first factor tends to zero at low temperatures for $\Delta k \to 0$ and saturates at large $\Delta k$. As a result $\omega^2(k)$ is very small at $\Delta k = 0$ causing the approximate touching of the two branches at $\omega = \omega_R$ and $\Delta k = 0$. With increasing $\Delta k$ $\omega^2(k)$ increases strongly leading to a downward dispersion of the lower branch even if $\omega_R$ was practically dispersionless as in our case. According to fig. 3 the upper branch increases at large $|\Delta k|$ roughly as $0.6J|\Delta k|$, i.e., with an effective spin wave velocity which is reduced by about a factor $2-3$ compared to spin wave theory similar as in experiment [2,3].

Using the same parameters as in figs. 2 and 3, fig. 4 shows $\chi''$ as a function of $H$ with the frequency as a parameter. As suggested by fig. 3, $\chi''$ exhibits a hourglass dispersion with intensities which are largest near $\omega_R$ and decay towards lower and higher frequencies. This decay is mainly due to the rapid decrease of $\chi(k)$ away from the antiferromagnetic wave vector $Q$. Figure 5 shows $\chi''$ as a function of $\omega$ for a fixed $H$ as a parameter. For dämpings $\eta$ of about 0.002 or smaller the main peak at $H = 0.5$ splits into a double peak due to the small gap between

Fig. 2: (Color online) $1 + M^{\text{RPA}}(Q, \omega)/\omega$ (solid and dotted lines) and $-M'(Q, \omega)/\omega$ (dash-dotted and dashed lines) as a function of frequency for two momenta $H$. Squares and circles denote poles of $\chi(k, \omega)$.

Fig. 3: (Color online) Position of the poles of $\chi(k, \omega)$ as a function of momentum. The shadowed region marks the particle-hole continuum.
Intensity. If one puts the double peak splits into two peaks which disperse Q upper and lower branch shown in fig. 3. Moving away from momentum at zero temperature as a function of frequency for different frequencies.

Fig. 4: (Color online) Imaginary part of the spin susceptibility at zero temperature as a function of momentum for different frequencies.

Fig. 5: (Color online) Imaginary part of the spin susceptibility at zero temperature as a function of frequency for different momenta.

The upper and lower branch shown in fig. 3. Moving away from Q the double peak splits into two peaks which disperse up- and downwards in frequency loosing at the same time intensity. If one puts $M = 0$ only the lower, weaker peak is obtained. This shows that the lower branch of spin excitations originates from the resonance state whereas the upper branch describes mainly local spin rotations.

The presented theory does not take into account correlation effects from static or dynamic stripes. This assumption seems to be reasonable in systems like YBCO or Bi2212 where stripes are usually not considered to be important. The experimental data in figs. 1 and 2 of ref. [2] and of figs. 2 and 3 of ref. [3] indeed agree at least qualitatively with our figs. 3 and 4. Whether our theory can also be applied to 214 cuprates [5,6] is not clear. It is conceivable that different input parameters than those used for YBCO yield a larger gap between the upper and the lower branch similar to that observed in $\text{La}_{1.84}\text{Sr}_{0.16}\text{CuO}_4$, see fig. 3a in ref. [6]. Our theory would then suggest that the lower branch originates in this case from a broad RPA resonance [21] whereas the upper branch is due to spin-wave–like excitations. This is exactly the picture put forward in ref. [6]. On the other hand, there is good evidence that stripes play a role in 214 cuprates. It also has been shown that the spin excitations atop on static [8,9] or dynamic stripes [10] have a hourglass-like dispersion so that the correct explanation of the data in this case remains unclear.

In conclusion, we have shown that the memory function of the spin susceptibility contains in general two distinct contributions due to RPA-like and due to rotational spin fluctuations. The first one dominates at large, the second one at small dopings. At intermediate dopings both are of similar magnitude which leads to one upwards and one downwards dispersing branch of excitations. At low temperatures the two branches are approximately degenerate at Q which explains, at least qualitatively, the observed hourglass dispersion at intermediate dopings.

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