BOGOLIUBOV QUASIPARTICLES COUPLED TO SPIN FLUCTUATIONS

In a superconductor the interaction of Bogoliubov quasiparticles with the spin degrees of freedom leads to inelastic scattering processes, in which a quasiparticle of momentum $\boldsymbol{k}$ and energy ω is scattered to a state with momentum $\boldsymbol{k}-\boldsymbol{q}$ and energy $\omega-\Omega$ through emission of a spin excitation with quantum numbers $(\boldsymbol{q},\Omega)$. These processes induce a damping of the quasiparticles—reflected mathematically by an increase of the imaginary part of the self-energy $\Sigma(\boldsymbol{k},\omega)$—and a redistribution of the spectral weight—encoded in the real part of the self-energy. The minimal model to describe the effects of such an interaction is [1, 2]

$$\hat{\Sigma}(\boldsymbol{k},i\omega_n)=\frac{g^2}{\beta}\sum_{\boldsymbol{q}\Omega_n}\hat{\mathscr{G}}_0(\boldsymbol{k}-\boldsymbol{q},i\omega_n-i\Omega_n)\chi_s(\boldsymbol{q},i\Omega_n), \tag{1}$$

which is the leading term of the perturbation theory in the electron-spin coupling. $\hat{\Sigma}$ and $\hat{\mathscr{G}}_0$ are 2×2 Nambu matrices and $\hat{\mathscr{G}}_0$ is the BCS Green's function in the absence of coupling. χ_s is the spin susceptibility, g is the coupling parameter, $\beta=(k_{\mathrm{B}}T)^{-1}$ is the inverse temperature, $i\omega_n$ and $i\Omega_n$ are the fermionic and bosonic Matsubara frequencies, respectively. Following Refs. 1 and 2 we use a phenomenological expression for χ_s in the superconducting state, assuming that (i) in the energy range of interest, namely below ~ 150 meV, the spin response is dominated by a sharp resonance at energy Ω_s near the antiferromagnetic vector $\boldsymbol{Q}=(\pi/a,\pi/a)$ of the two-dimensional Brillouin zone, and (ii) in the region of $\boldsymbol{q}$ space where the resonance is present, its dispersion away from $\boldsymbol{q}=\boldsymbol{Q}$ is small enough that it can be neglected. Such assumptions are guided by the experimental results of inelasting neutron scattering [3, 4] (INS), and they allow one to separate the frequency and momentum dependencies of the spin susceptibility as

$$\chi_s(\boldsymbol{q},\omega)=-\frac{W_s}{\pi}F(\boldsymbol{q})\int d\varepsilon\,\frac{I(\varepsilon)}{\omega-\varepsilon+i0^+}. \tag{2}$$

We choose the functions $F(\boldsymbol{q})$ and $I(\omega)$ such that $\sum_{\boldsymbol{q}}F(\boldsymbol{q})=\int_0^\infty d\omega\,I(\omega)=1$. Therefore W_s stands for the momentum and frequency integrated spectral weight of the resonance: $W_s=\sum_{\boldsymbol{q}}\int_0^\infty d\omega\,\mathrm{Im}\,\chi_s(\boldsymbol{q},\omega)$. The function $F(\boldsymbol{q})$ is written as a Lorentzian of with Δq (HWHM) peaked at $\boldsymbol{q}=\boldsymbol{Q}$:

$$F(\boldsymbol{q})=\frac{F_0}{\sin^2\left(\frac{q_x-Q_x}{2}\right)+\sin^2\left(\frac{q_y-Q_y}{2}\right)+(\Delta q/4)^2}, \tag{3}$$

where the constant F_0 ensures the normalization of $F(\boldsymbol{q})$. The energy distribution $I(\varepsilon)$ measured by inelastic neutron scattering is resolution-limited in YBCO [5], which suggests that the resonance is infinitely sharp [1, 2]: $I(\varepsilon)=\delta(\varepsilon-\Omega_s)-\delta(\varepsilon+\Omega_s)$. Here we use a slightly more general form,

$$I(\varepsilon)=I_0\left[L_{\Gamma_s}(\varepsilon-\Omega_s)-L_{\Gamma_s}(\varepsilon+\Omega_s)\right], \tag{4}$$

where $L_\Gamma(\varepsilon)=(\Gamma/\pi)/(\varepsilon^2+\Gamma^2)$ is the Lorentzian and I_0 ensures the normalization of $I(\varepsilon)$. The form Eq. (4) allows one to take into account a possible finite lifetime $\tau_s\sim\Gamma_s^{-1}$ of the spin excitation. Indeed the INS measurements indicate that the resonance is somewhat broader in Bi2212 (Ref. 4) and Bi2223 (Ref. 6) than in YBCO, and would be consistent with $\Gamma_s\approx 6$ meV. Alternatively, Eq. (4) can be regarded as a crude way to account for the dispersion of the resonance observed experimentally in YBCO [7, 8], which would broaden the sharp mode into a band of width Γ_s.

It is convenient to express the Green's function $\hat{\mathscr{G}}_0$ in Eq. (1) using the spectral representation:

$$\hat{\mathscr{G}}_0(\boldsymbol{k},\omega)=\int d\varepsilon\,\frac{\hat{A}(\boldsymbol{k},\varepsilon)}{\omega-\varepsilon}. \tag{5}$$

In an ideal BCS d-wave superconductor the spectral function would be simply $\hat{A}(\boldsymbol{k},\varepsilon)=\hat{u}_{\boldsymbol{k}}\delta(\varepsilon-E_{\boldsymbol{k}})+\hat{v}_{\boldsymbol{k}}\delta(\varepsilon+E_{\boldsymbol{k}})$ where

$$\hat{u}_{\boldsymbol{k}}=\frac{1}{2}\begin{pmatrix}1+\frac{\xi_{\boldsymbol{k}}}{E_{\boldsymbol{k}}} & \frac{\Delta_{\boldsymbol{k}}}{E_{\boldsymbol{k}}}\\ \frac{\Delta_{\boldsymbol{k}}}{E_{\boldsymbol{k}}} & 1-\frac{\xi_{\boldsymbol{k}}}{E_{\boldsymbol{k}}}\end{pmatrix},\quad \hat{v}_{\boldsymbol{k}}=\mathbb{1}-\hat{u}_{\boldsymbol{k}}, \tag{6}$$

and $E_{\boldsymbol{k}}=\sqrt{\xi_{\boldsymbol{k}}^2+|\Delta_{\boldsymbol{k}}|^2}$ with $\xi_{\boldsymbol{k}}$ the electron dispersion and $\Delta_{\boldsymbol{k}}=\frac{\Delta_0}{2}(\cos k_x-\cos k_y)$ the superconducting gap. Like for the spin excitations, we wish to allow for a finite lifetime of the Bogoliubov quasiparticles due, *e.g.*, to impurity scattering, and we introduce an additional scattering rate Γ via a self-energy term $\Sigma_{\text{imp}}(\omega) = -i\Gamma\,\text{sign}[\text{Im}(\omega)]$. This constant scattering rate amounts to replace the delta functions in the BCS spectral function by Lorentzian functions:

$$\hat{A}(\boldsymbol{k},\varepsilon) = \hat{u}_{\boldsymbol{k}} L_{\Gamma}(\varepsilon - E_{\boldsymbol{k}}) + \hat{v}_{\boldsymbol{k}} L_{\Gamma}(\varepsilon + E_{\boldsymbol{k}}). \tag{7}$$

Inserting Eqs (2) and (5) into Eq. (1) one can perform the summation over Matsubara frequencies, and using Eqs (4) and (7) one obtains the self-energy on the real-frequency axis:

$$\hat{\Sigma}(\boldsymbol{k},\omega) = \alpha^2 \sum_{\boldsymbol{q}} F(\boldsymbol{q})[\hat{u}_{\boldsymbol{k}-\boldsymbol{q}} B(\omega, E_{\boldsymbol{k}-\boldsymbol{q}}) + \hat{v}_{\boldsymbol{k}-\boldsymbol{q}} B(\omega, -E_{\boldsymbol{k}-\boldsymbol{q}})], \tag{8}$$

where we have introduced the dimensionless coupling constant $\alpha^2 = (g/\Lambda)^2 W_s I_0/\pi$ with Λ a characteristic energy scale of the model, which we take as the nearest-neighbor hopping t_1. For definiteness the function B is written down explicitly in the Appendix. From the self-energy (8) one can compute the full propagator $\hat{\mathscr{G}}$ using the Dyson equation, $\hat{\mathscr{G}}^{-1} = \hat{\mathscr{G}}_0^{-1} - \hat{\Sigma}$. The first component is given by

$$\mathscr{G}_{11}(\boldsymbol{k},\omega) = \frac{1}{\omega - \xi_{\boldsymbol{k}} + i\Gamma - \Sigma_{11}(\boldsymbol{k},\omega) - \frac{[\Delta_{\boldsymbol{k}} + \Sigma_{12}(\boldsymbol{k},\omega)]^2}{\omega + \xi_{\boldsymbol{k}} + i\Gamma - \Sigma_{22}(\boldsymbol{k},\omega)}}, \tag{9}$$

and directly provides the one-particle density of states $N(\omega) = \sum_{\boldsymbol{k}} \left(-\frac{1}{\pi}\right) \text{Im}\,\mathscr{G}_{11}(\boldsymbol{k},\omega)$. The different roles of the various components of the matrix $\hat{\Sigma}$ are obvious in Eq. (9): Σ_{11} and Σ_{22} renormalize the quasiparticle dispersion on the electron and hole branches, while Σ_{12} renormalizes the gap $\Delta_{\boldsymbol{k}}$. Finally, using the tunneling matrix element calculated by Tersoff and Hamann [9] for the STM junction, the STM tunneling conductance reads [10]

$$\frac{dI}{dV} \propto \int d\omega_1 d\omega_2\, N(\omega_1)[-f'(\omega_1 - \omega_2)] g_{\sigma}(\omega_2 - eV). \tag{10}$$

f' denotes the derivative of the Fermi function, and we also applied a Gaussian filtering function g_σ of width σ, in order to mimic the finite experimental resolution.

At this point the model contains six parameters: the spin-resonance energy Ω_s, its width in energy Γ_s, and momentum Δq, a coupling constant α, the scattering rate Γ, and the d-wave gap amplitude Δ_0. We still have to parametrize the bare dispersion $\xi_{\boldsymbol{k}}$. We use a tight-binding dispersion with up to five neighbor hoppings (setting the lattice parameter $a \equiv 1$):

$$\begin{aligned}\xi_{\boldsymbol{k}} = 2t_1(\cos k_x + \cos k_y) + 4t_2 \cos k_x \cos k_y + 2t_3(\cos 2k_x + \cos 2k_y) +& \\ 4t_4(\cos 2k_x \cos k_y + \cos k_x \cos 2k_y) + 4t_5 \cos 2k_x \cos 2k_y - \mu.&\end{aligned} \tag{11}$$

It should be noted that the precise values of the hoppings t_i have little impact on the final STM spectrum Eq. (10), except for one particular property, namely the energy of the van-Hove singularity with respect to the chemical potential. The latter is due to the saddle point of the dispersion at the point $\text{M} = (\pi, 0)$ of the Brillouin zone, where the bare energy is

$$\xi_{\text{M}} = -4(t_2 - t_3 - t_5) - \mu. \tag{12}$$

THE FUNCTION $B(\omega, E)$

From Eqs (1) to (7) it results that the function $B(\omega, E)$ entering Eq. (8) is

$$B(\omega, E) = \Lambda^2 \int d\varepsilon_1 d\varepsilon_2 \frac{L_{\Gamma}(\varepsilon_1 - E)[L_{\Gamma_s}(\varepsilon_2 - \Omega_s) - L_{\Gamma_s}(\varepsilon_2 + \Omega_s)][1 - f(\varepsilon_1) + b(\varepsilon_2)]}{\omega - \varepsilon_1 - \varepsilon_2 + i0^+}, \tag{13}$$

where f and b are the Fermi and Bose functions, respectively. Changing variables this can be rewritten as

$$\begin{aligned}\Lambda^{-2} B(\omega, E) = \int dx\, L_{\Gamma}(x) \int dy \frac{L_{\Gamma_s}(y)}{\omega - E - \Omega_s - x + i0^+ - y} - \int d\varepsilon_1\, L_{\Gamma}(\varepsilon_1 - E) f(\varepsilon_1) \int dy \frac{L_{\Gamma_s}(y)}{\omega - \Omega_s - \varepsilon_1 + i0^+ - y} \\ + \int d\varepsilon_2\, L_{\Gamma_s}(\varepsilon_2 - \Omega_s) b(\varepsilon_2) \int dx \frac{L_{\Gamma}(x)}{\omega - E - \varepsilon_2 + i0^+ - x} - \{\Omega_s \to -\Omega_s\}.\end{aligned}$$

Using the identity $\int dx\, L_\Gamma(x)/(z-x) = 1/[z + i\Gamma\,\mathrm{sign}(\mathrm{Im}\, z)]$ we have

$$\Lambda^{-2}B(\omega,E) = \frac{1}{\omega - E - \Omega_s + i(\Gamma+\Gamma_s)} - \int d\varepsilon_1\, \frac{L_\Gamma(\varepsilon_1 - E)f(\varepsilon_1)}{\omega - \Omega_s + i\Gamma_s - \varepsilon_1} + \int d\varepsilon_2\, \frac{L_{\Gamma_s}(\varepsilon_2 - \Omega_s)b(\varepsilon_2)}{\omega - E + i\Gamma - \varepsilon_2} - \big\{\Omega_s \to -\Omega_s\big\}.$$

The remaining integrals can be performed by closing the integration contour in the complex plane. Due to the poles of the Fermi and Bose functions at the frequencies $i\omega_n$ and $i\Omega_n$, respectively, the integrals involve infinite sums of the residue of these poles. These sums can be rewritten in terms of the digamma function

$$\psi(x) = \lim_{N\to\infty}\left(\ln N - \sum_{n=0}^{N}\frac{1}{n+x}\right).$$

We quote only the final result:

$$\begin{aligned}\Lambda^{-2}B(\omega,E) =& \frac{1 - f(E - i\Gamma) + b(\Omega_s - i\Gamma_s)}{\omega - E - \Omega_s + i(\Gamma+\Gamma_s)} + \frac{\Gamma}{\pi}\frac{\psi\left(\frac{1}{2} + \frac{\beta\Gamma_s}{2\pi} + \frac{\beta(\omega-\Omega_s)}{2\pi i}\right)}{(\omega - E - \Omega_s + i\Gamma_s)^2 + \Gamma^2} + \frac{\Gamma_s}{\pi}\frac{\psi\left(\frac{\beta\Gamma}{2\pi} + \frac{\beta(\omega-E)}{2\pi i}\right)}{(\omega - E - \Omega_s + i\Gamma)^2 + \Gamma_s^2}\\ &+ \frac{1}{2\pi i}\left[\frac{\psi\left(\frac{1}{2} - \frac{\beta\Gamma}{2\pi} + \frac{\beta E}{2\pi i}\right) + \psi\left(-\frac{\beta\Gamma_s}{2\pi} + \frac{\beta\Omega_s}{2\pi i}\right)}{\omega - E - \Omega_s + i(\Gamma+\Gamma_s)} - \frac{\psi\left(\frac{1}{2} + \frac{\beta\Gamma}{2\pi} + \frac{\beta E}{2\pi i}\right)}{\omega - E - \Omega_s - i(\Gamma-\Gamma_s)} - \frac{\psi\left(\frac{\beta\Gamma_s}{2\pi} + \frac{\beta\Omega_s}{2\pi i}\right)}{\omega - E - \Omega_s + i(\Gamma-\Gamma_s)}\right]\\ &- \big\{\Omega_s \to -\Omega_s\big\}.\end{aligned} \tag{14}$$

The function B simplifies considerably in the case of a sharp mode ($\Gamma_s = 0^+$) and sharp quasiparticles ($\Gamma = 0^+$) as well as zero temperature:

$$B(\omega,E) = \frac{\Lambda^2}{\omega - E - \Omega_s\,\mathrm{sign}(E) + i0^+} \qquad (\Gamma_s = \Gamma = T = 0), \tag{15}$$

as can be readily deduced from Eq. (13) by replacing the Lorentzians by delta functions.

[1] M. Eschrig and M. R. Norman, Phys. Rev. Lett. **85**, 3261 (2000).
[2] J.-X. Zhu, A. V. Balatsky, T. P. Devereaux, Q. Si, J. Lee, K. McElroy, and J. C. Davis, Phys. Rev. B **73**, 014511 (2006).
[3] H. A. Mook, M. Yethiraj, G. Aeppli, T. E. Mason, and T. Armstrong, Phys. Rev. Lett. **70**, 3490 (1993).
[4] H. F. Fong, P. Bourges, Y. Sidis, L. P. Regnault, A. Ivanov, G. D. Gu, N. Koshizuka, and B. Keimer, Nature **398**, 588 (1999).
[5] J. Rossat-Mignod, L. P. Regnault, C. Vettier, P. Bourges, P. Burlet, J. Bossy, J. Y. Henry, and G. Lapertot, Physica C **185**, 86 (1991).
[6] S. Pailès, Ph.D. thesis, Université Paris 6 (2004).
[7] P. Bourges, Y. Sidis, H. F. Fong, L. P. Regnault, J. Bossy, A. Ivanov, and B. Keimer, Science **288**, 1234 (2000).
[8] D. Reznik, P. Bourges, L. Pintschovius, Y. Endoh, Y. Sidis, T. Masui, and S. Tajima, Phys. Rev. Lett. **93**, 207003 (2004).
[9] J. Tersoff and D. R. Hamann, Phys. Rev. Lett. **50**, 1998 (1983).
[10] Ø. Fischer, M. Kugler, I. Maggio-Aprile, C. Berthod, and C. Renner, Rev. Mod. Phys. **79**, 353 (2007).