Relaxation Models for Cuprate NMR

From the very beginning of cuprate NMR studies, it was clear that understanding the relaxation properties for all sites with nuclear spin species would be a major challenge for theorists and experimentalists alike. In Chap. 3 the Mila-Rice-Shastry model [1,2] was presented, including the quantum-chemical basis for transferred HF couplings and the spin Hamiltonian treatment of local spin and orbital HF effects at the Cu$^{2+}$ sites. With the latter formulation a complete characterization of the NMR shift tensors for YBCO7 and YBCO6.63 has been carried out in Chaps. 3 and 4. Then, using general expressions for $1/T_1$, Mila and Rice discussed $T_1$ anisotropy for $^{63}$Cu(2) in YBCO7 (Sect. 3.3.4). A simplified model given in Sect. 4.1.2 offered an interpretation of $T_1$ anisotropies and spin correlation effects for the $^{89}$Y and $^{17}$O(2,3) sites. These developments set the stage for the most serious challenge, which is the locally-varying, overall temperature dependences of the $T_1$ processes in these compounds. Such a panorama of complex relaxation behavior had never been encountered before the cuprates were discovered.

A variety of models treating the relaxation processes have been put forward in the literature. Here, we will review the results of several of these models in an effort to gauge the present status of our understanding of these matters. There have been phenomenological models put forward by Monien and Pines [3] and Millis, Monien, and Pines [4,5], where the AFM fluctuations are taken into account by means of an RPA treatment of the AFM exchange interactions. Moreover, it is assumed and is consistent with experiment that the Cu$^{2+}$ spin variables are itinerant and undergo pairing in the superconducting state. Similar modeling along these lines has also been put forward by Horvatić et al. [6].

These models were presented early on and gave a reasonable account of the data which were available at the time. In particular, they met the challenge of explaining the behavior of all measured relaxation processes with a single dynamical variable per Cu site, and did so using only HF couplings generated by the Cu$^{2+}$ spin moments, in a picture consistent with the Mila-Rice model [1] of on-site spin–Hamiltonian and transferred HF couplings of the general
form $\sum_A A_\alpha S_\alpha I_\alpha$. A possible deviation from this form may occur in the case of $^{89}\text{Y}$ in YBCO compounds, where the transferred coupling is very weak and the dipolar interactions, which do not have the latter form, come into play.

A slightly different approach to modeling the dynamical susceptibility has been pursued by Auler et al., [7], where the basic form of the dynamic susceptibility was taken directly from INS data. This scenario had the unusual feature that the range of spin-spin correlations was fixed, although their strength certainly increased as temperature was lowered. These authors also made the unusual step of using spin-echo decay time ($T_2g$) measurements to determine the strength of the AFM susceptibility peak. In reviewing the results of their analysis, we shall find that a satisfactory account of the data can be achieved in this fashion.

Beyond phenomenology, there have also been first-principles model calculations by Bulut and Scalapino [8] and by Si, Levin, and co-workers [9]. The latter are, of course, more difficult to formulate and execute, but these have yielded impressive insights. Finally, there has been a proposal by Varma which departs from the usual spin HF-only picture wherein an intersite orbital matrix element is suggested to make an important contribution to the Cu(2)-site relaxation process [10]. The essence of these various results will be summarized below.

This chapter will begin, however, with a discussion of the characterization of the cuprate relaxation properties developed quite recently by Uldry and Meier [11] (UM). This is a scheme of a fairly general nature for characterizing the spin dynamics and spin-spin correlations which determine the relaxation behavior in the CuO$_2$ planes. It serves as a useful framework for evaluating almost any experimental data or theoretical model.

### 5.1 The Uldry-Meier Parameterization Model

The Uldry-Meier (UM) approach to the analysis of cuprate relaxation data relies only on a general formulation of spin-fluctuation $T_1$ processes, which is characterized by just three elements, (i) the HF constants, (ii) real-space, dynamical spin-spin correlation coefficients, and (iii) an effective correlation time parameter in which the temperature variation of the spin dynamics is also implicit in a very general way. The HF parameters used are those derived from the Mila-Rice-Shastry model [3.3.2] for each site in and near the CuO$_2$ planes. The spin-spin correlations and correlation time which characterize the relaxation processes are assumed to apply to all nuclear species considered, e.g. the $^{63}\text{Cu}(2)$, $^{17}\text{O}(2,3)$, and the $^{89}\text{Y}$ in YBCO7 and YBCO6.63, etc. The spin-spin correlations are allowed to be anisotropic, but the correlation time variable is assumed to be isotropic and common to all spin fluctuation processes. After describing the UM analysis, the broader significance of this methodology will be discussed at the end of this section.

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1 The Cu(1) sites and environs in YBCO are set aside as a separate problem.