Chapter 1

NORMAL STATE PROPERTIES OF CUPRATES:
t-J MODEL VS. EXPERIMENT

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Abstract

We discuss some recent results for the properties of doped antiferromagnets, obtained within the planar t-J model mainly by the finite-temperature Lanczos method, with the emphasis on the comparison with experimental results in cuprates. Among the thermodynamic properties the chemical potential and entropy are considered, as well as their relation to the thermoelectric power. At the intermediate doping model results for the optical conductivity, the dynamical spin structure factor and spectral functions reveal a marginal Fermi-liquid behaviour, close to experimental findings. It is shown that the universal form of the optical conductivity follows quite generally from the overdamped character of single-particle excitations.

1. INTRODUCTION

It is by now quite evident through numerous experiments on electronic properties that cuprates, being superconductors at high temperatures, are also strange metals in the normal phase [1]. On the other hand it also appears that most features can be well represented by prototype single-band models of correlated electrons, as the Hubbard model and the t-J model. In spite of their apparent simplicity these models are notoriously difficult to treat analytically, in particular in the most interesting regime of strong correlations. This has led to intensive efforts towards numerical approaches [2], mostly using quantum Monte Carlo (QMC) and the exact diagonalization (ED) methods.

The subject of this contribution is the planar t-J model (Hubbard model is expected to show similar behaviour in the strong correlation regime), which represents layered cuprates as doped antiferromagnets (AFM) and within a
single band both mobile charges and spin degrees of freedom,

\[ H = -t \sum_{\langle ij \rangle} \langle \tilde{c}^\dagger_{js} \tilde{c}_{is} + \text{H.c.} \rangle + J \sum_{\langle ij \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j). \]  \hspace{1cm} (1.1)

Strong correlations are here imposed by strictly forbidding doubly occupied sites. So far most calculations were performed for the ground state at \( T = 0 \), where the standard Lanczos algorithm offers an efficient exact-diagonalization analysis of small systems [2]. More recently a novel numerical method, finite-temperature Lanczos method (FTLM) [3, 4], has been introduced combining the Lanczos method with a random sampling, which allows for an analogous treatment of static and dynamic properties at \( T > 0 \).

One of most important conclusion of experimental efforts in the last decade is the realization that the electronic phase diagram in the parameter space of planar hole concentration \( c_h \) and temperature \( T \) is quite universal. Materials are usually classified as underdoped, optimally doped and overdoped, with respect to the highest \( T_c \) in a given class. In our analysis we cannot establish the superconductivity, so we will use the highest entropy (at low \( T \)) as a criterion for the optimum doping. In fact both criteria are quite close for real cuprates [5] and one could conjecture that this relation is not accidental. In particular since in thermodynamic quantities at the same doping also the pseudogap scale disappears.

In this contribution we mainly discuss two topics related to the normal-state properties of cuprates. In Sec.II we deal with the thermodynamic quantities: entropy, chemical potential and closely related thermoelectric power, all of them in the full range of \( c_h \). In Sec.III we concentrate on the appearance and the relation between different manifestations of the marginal-Fermi-liquid (MFL) behaviour, observed in the optical conductivity, dynamic spin susceptibility and spectral functions at the intermediate (optimum) doping.

### 2. THERMODYNAMICS

Let us first consider thermodynamic quantities, which can be directly derived from the grand-canonical sum: free energy density \( \mathcal{F} \), chemical potential \( \mu \) and entropy density \( s \). For these the FTLM is particularly simple to implement [6, 4], since it requires only a minor generalization of the usual Lanczos method. Results presented below were obtained mostly for \( N = 20 \) sites and parameters \( J/t = 0.3 \), corresponding to the situation in cuprates (where \( t \sim 0.4 \text{eV} \)). Note that in small systems only results above certain (size dependent) \( T \) are meaningful, i.e. in cases below typically \( T > T_{fs} \sim 0.1 \ t \).

Let us first discuss results for \( s \), shown in Fig.(1.1) for various \( T \). It seems quite generic feature of such a system that \( s(c_h) \) exhibits a (rather broad) maximum at the intermediate doping \( c_h \sim c_h^* \). The increase of \( s \) on doping
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Figure 1.1 $s \text{ vs. } c_h$ at several $T$ [4]. For comparison also experimental results for LSCO [5] at highest $T = 320 \, K \sim 0.07 \, t$ are shown.

can be plausibly related to the frustration between the AFM exchange $\propto J$ and the hole kinetic energy $\propto c_h t$ preferring the FM configuration. This naturally leads to a most frustrated situation at $c_h^* \sim J/t$. It is quite fortunate that the FTLM works best, i.e. $T_{fs}$ is lowest, just in the cases with large $s$ and large frustration, while other methods have difficulties in such situation. E.g. QMC is plagued with the minus-sign problem which seems to be intimately related to fermionic frustration.

Even more surprising fact is the magnitude of $s$ at $T < J$. E.g. at $T = 0.1 \, t$ at $c_h^*$ we get 40% of $s(T = \infty)$. Clearly we are dealing with a system which has very low degeneracy (Fermi) temperature $T_{deg} < J$, far below the free fermion value $T_{deg}^0 \sim 8t$. Such a conclusion is in agreement with experiments in cuprates. In recent years $s$ has been measured in YBCO and LSCO (also presented in Fig.(1.1) in a wide doping regime [5] and our results show good quantitative agreement.

For $\mu_h(T)$, presented in Fig.(1.2), we mostly do not find a $T^2$ dependence of $\mu_h$ at low $T$, as expected for a normal Fermi liquid, except within the extremely overdoped regime $c_h \geq 0.3$. In particular, in a broad range $0.05 < c_h < 0.3$ we find a roughly linear variation $\mu_h(T) = \mu_h(T = 0) + \alpha k_B T$, whereby the slope $\alpha$ changes the sign at $c_h = c_h^* \sim 0.15$. The variation $\mu(c_h)$ at low $T$ has been recently deduced experimentally from the shift of photoemission spectroscopy spectra in LSCO [7], and the agreement with our results is quite satisfactory [4]. From photoemission results as well as from our Fig.(1.2) it is also evident
that \( \mu(\text{ch} < \text{ch}^*) \) is very flat which would indicate that at \( T \to 0 \) and \( \text{ch} < \text{ch}^* \) the compressibility \( \kappa \propto -d\text{ch}/d\mu \) is very large or even diverging, as would e.g. follow from the phase separation scenario [8] or the singular \( \text{ch} \to 0 \) limit [1]. It should be however stressed that the distinction between these scenarios could be relevant only at very low \( T \ll J \), since both experiment and numerics indicate on quite large \( s \), i.e. a distribution over a wide spectrum of states, even at \( T \sim J/10 \).

It is quite helpful to realize that the free energy density \( \mathcal{F}(\text{ch}, T) \) relates the variation of \( s = \partial \mathcal{F}/\partial T \) and \( \mu = \partial \mathcal{F}/\partial \text{ch} \), i.e.\[
\frac{\partial s}{\partial \text{ch}} \bigg|_T = -\frac{\partial \mu}{\partial T} \bigg|_{\text{ch}} = \frac{\partial^2 \mathcal{F}}{\partial \text{ch} \partial T}.
\] (1.2)

This connects the maximum \( s(\text{ch}^*) \) with the change in slope \( d\mu_\text{h}(\text{ch}^*)/dT = 0 \). Moreover Eq.(1.2) allows us to discuss more confidently the slope \( d\mu_\text{h}/dT = \alpha k_B \) for which we find in the underdoped regime \( \alpha \sim 2 \). Although the latter has not been so far verified directly for cuprates, one can extract in the same regime from the measured \( \partial s/\partial \text{ch} \) for LSCO and YBCO at \( T > 100 K \) similar values \( \alpha > 1 \) [5]. It is quite evident that at \( \alpha > 1 \) we are not dealing with a degenerate Fermi liquid but rather with the nondegenerate doped carriers, which is a situation typical for a doped (nondegenerate) semiconductor. One
should just recall the standard expression for $\mu_h$ in p-type semiconductor,

$$c_h = P_v e^{-(\epsilon_v - \mu_h)/k_BT} = \mathcal{P} \ln \frac{P_v}{c_h} > k_B,$$

where in our notation $P_v \sim 1$. The constant slope $d\mu_h/dT$ observed in our calculations down to $T < 0.1$ $t$ is a confirmation of such a picture. In experimental results for $s$ one should however notice a reduction of $\alpha$ with $T$, but even at $T \sim T_c$ the system is not evidently a normal Fermi liquid with $\alpha < 1$.

Another consequence of such a semiconductor picture is an expression for the thermopower $S$,

$$S \sim \frac{\bar{\epsilon} - \mu_h(T)}{e_0T} \sim \frac{\mu_h(T = 0) - \mu_h(T)}{e_0T} \sim \alpha S_0,$$

where $S_0 = k_B/e_0 = 86\mu V/K$. The validity of this approximation we have verified within the $t$-$J$ model also directly by evaluating the mixed current-energy current correlation function and observing that they are proportional to the current-current correlation $C_{J,EJ}(\omega) = \mu_h(0)C(\omega)$. The result is in Fig.(1.3) is good agreement with the general experimental observation in cuprates [9] of a large and rather $T$-independent $S$ at low doping. In fact instead of the usual semiconductor expression for $\alpha$ at $c_h \ll 1$, Eq.(1.4), in a strongly correlated system it is more appropriate to use the proper statistics for
the $t$-$J$ model leading to $\alpha \sim \ln[2(1 - c_h)/c_h]$, which even predicts the change of sign at $c_h \sim 0.3$.

3. DYNAMICS AT OPTIMUM DOPING

It has been quite early established from experiments that cuprates in the normal state do not follow the behaviour consistent with the normal Fermi liquid. In contrast several static and dynamic quantities at optimum doping can be quite well accounted for within the marginal Fermi liquid (MFL) concept [10]. Most evident example is the dynamic conductivity $\sigma(\omega)$ which does not obey the usual Drude form with a constant rate $1/\tau$ but can be well fitted in a broad range of $\omega, T$ with the generalized MFL form $\tau^{-1}(\omega, T) = \lambda(\omega + \eta T)$, describing also the well established linear resistivity law $\rho \propto T$. It has been natural to postulate an analogous MFL behaviour for quasiparticle (QP) relaxation in spectral functions as e.g. measured by the angle-resolved photoemission spectroscopy (ARPES). Only recently, however, the high resolution ARPES experiments on BSCCO [11] seem to be in position to confirm beyond doubt this behaviour, obeyed in the optimum-doped materials surprisingly even at $T < T_c$ for QP along the nodal direction in the Brillouin zone. Most evident indication that also spin dynamics follows the MFL concept is the observed anomalous NMR and NQR spin-lattice relaxation rate $1/T_1(T) \sim \text{const.}$ [12] instead of usual Korringa law in metals.

By calculating using FTLM several related quantities, describing charge and spin dynamics within the $t$-$J$ model, we established that the MFL concept applies well in a broad range of intermediate hole doping $0.1 < c_h < 0.3$. We discuss here in particular the dynamical conductivity $\sigma(\omega)$, the local spin susceptibility $\chi_L(\omega)$ [13] and the QP relaxation rate as obtained from the analysis of spectral functions $A(k, \omega)$ [14]. Moreover, $\sigma(\omega)$ has been been found close to a universal form [13],

$$\sigma(\omega) = C_0 \frac{1 - e^{-\omega/k_B T}}{\omega},$$

in a remarkably broad frequency regime $0 < \omega < \omega^* \sim 2t$, while $C_0$ is essentially $T$-independent for $T < J$. Resulting $\sigma(\omega < \omega^*)$ is clearly governed by $T$ only. Evidently, Eq.(1.5) reproduces the linear resistivity law $\rho = T/C_0$ and is consistent with the MFL scenario for $\tau^{-1}(\omega, T)$, however in a very restrictive way since both MFL parameters are essentially fixed. A reasonable overall fit can be e.g. achieved by $\lambda \sim 0.6$ and $\eta \sim 2.7$. When optical experiments on $\sigma(\omega)$ in cuprates are analysed within the MFL framework quite close values for $\lambda, \eta$ are in fact reported [15, 16]. In addition, the model results reproduce well also the absolute value of $\sigma(\omega)$ and $\rho(T)$ [4].

Analogous universality has been found also in the spin dynamics, in particular when looking at the local spin susceptibility $\chi_L(\omega)$ and related spin
correlation function $S_L(\omega)$,

$$
\chi''_L(\omega) = \frac{1}{\pi} \tanh \left( \frac{\omega}{2T} \right) \bar{S}_L(\omega),
$$

(1.6)

where $\bar{S}_L(\omega) = S_L(\omega) + S_L(-\omega)$ is the symmetrized function, having a fixed sum rule

$$
\int_0^\infty \bar{S}(\omega) d\omega = \langle (S^z_i)^2 \rangle = \frac{1}{4} (1 - \chi_h).
$$

(1.7)

The most important message of numerical results on spin dynamics at intermediate doping is that $\bar{S}_L(\omega)$ is nearly $T$-independent in a broad range of $T$, in particular for $T < J$. Moreover $\bar{S}_L(\omega)$ is only weakly doping dependent consistent with the sum rule. So we have a conclusion that at intermediate doping the more fundamental and universal quantity is the correlation function $S_L(\omega)$ and not the susceptibility $\chi''_L(\omega)$, which is the analogy to the relation between $C(\omega)$ and $\sigma(\omega)$ in Eq.(1.5). For the spin dynamics this is also the message of the anomalous NMR $1/T_1$ in cuprates [12]. As a result $\chi''_L(\omega)$, Eq.(1.6), follows the MFL behaviour i.e. at $\omega < T$ one gets anomalous $T$ dependence $\chi''_L(\omega) \propto \omega/T$.

A MFL-type QP relaxation is extracted within the $t$-$J$ model also from the analysis of the spectral functions $A(k, \omega)$ near the optimum doping [14, 4]. For the characterization of QP properties the self energy $\Sigma(k, \omega)$ is crucial. On the other hand the same information can be also expressed in terms of QP parameters $Z_k, \Gamma_k, \epsilon_k$. Both definitions are related as

$$
A(k, \omega) = -\frac{1}{\pi} \text{Im} \frac{1}{\omega - \Sigma(k, \omega)} = \frac{1}{\pi} \frac{Z_k \Gamma_k}{(\omega - \epsilon_k)^2 + \Gamma_k^2}.
$$

(1.8)

For QP near the Fermi surface the hole-part self energy $\omega < 0$ is found to be of the MFL form, i.e. $\text{Im} \Sigma \sim -\tilde{\gamma}(\omega + \xi T)$ with $\tilde{\gamma} \sim 1.4$ and $\xi \sim 3.5$. $\tilde{\gamma} > 1$ means an overdamped character of QP, since the full width at half maximum $\Delta \sim 2\Gamma(\epsilon) > \epsilon$ is larger than the QP (binding) energy $\epsilon$. This should be contrasted with the electron-like regime $\omega > 0$ where the damping is found to be essentially smaller and consequently QP can be underdamped.

Here we comment on the relation of our results to recent ARPES results in BSCCO. The analysis for hole-like excitations in the nodal direction $(0, 0) - (\pi, \pi)$ shows the MFL form with the QP damping $\Gamma \sim 0.75\omega$ for $\omega > T$ and $\Gamma \sim 2.5T$ for $\omega < T$ [11]. This again means an overdamped character of hole excitations, since $2\Gamma(\epsilon) > \epsilon$. In making the comparison one should take into account that $\Gamma = Z|\text{Im} \Sigma|$. Since at the peak position we find $Z \sim 0.5$ experimental and model values appear reasonably close.

Let us finally discuss the relation of $\sigma(\omega)$ and the associated relaxation rate $1/\tau$ to the QP damping $\Gamma$ [17]. In the case of weak scattering one finds $1/\tau \sim 2\Gamma$. In cuprates as well as in the $t$-$J$ model we are apparently dealing with
overdamped QP, so the relation is at least questionable. Also, the conductivity form Eq.(1.5) appears to be universal, while the QP damping does not seem to be parameter free.

One approach is to approximate the current-current correlation function \( C(\omega) \), which in general replaces \( C_0 \) in Eq.(1.5), by a decoupling in terms of spectral functions \( A(k, \omega) \) neglecting possible vertex corrections, i.e.

\[
C(\omega) = \frac{2\pi e^2}{N} \sum_k (v_0^2) \int d\omega' f(-\omega') f(\omega'-\omega) A(k, \omega') A(k, \omega'-\omega). \tag{1.9}
\]

In order to reproduce the MFL form of \( \sigma(\omega) \) one has to assume the MFL form for the spectral function, Eq.(1.8), i.e. the QP damping of the form \( \Gamma = \gamma(|\omega| + \xi T) \). We neglect also the \( k \) dependence of \( \Gamma \) and \( Z \). In fact it is enough to assume that \( \Gamma_k(\omega) \) is independent of deviations \( \Delta_k \) perpendicular to the Fermi surface. The latter is just what is observed in recent ARPES studies of BSCCO [11]. Replacing in Eq.(1.9) the \( k \) summation with an integral over \( \epsilon \) with a slowly varying density of states we can derive

\[
\int d\epsilon A(\epsilon, \omega') A(\epsilon, \omega'-\omega) = \frac{Z^2}{\pi} \frac{\overline{\Gamma}(\omega, \omega')}{\omega^2 + \overline{\Gamma}(\omega, \omega')^2}, \tag{1.10}
\]

where \( \overline{\Gamma}(\omega, \omega') = \Gamma(\omega') + \Gamma(\omega'-\omega) \). We are thus dealing with a function \( C(\omega) \) depending only on the ratio \( \omega/T \), and on MFL parameters \( \gamma, \xi \). For \( \gamma \ll 1 \) we recover via such an analysis \( C(\omega) \) strongly peaked at \( \omega = 0 \) and consequently MFL-type \( \sigma(\omega) \) with \( 1/\tau(\omega) = 2\Gamma(\omega/2) \) [10]. No such simple relation is valid when one approaches the regime of overdamped QP excitations \( \gamma \sim 1 \) or more appropriate \( \gamma \xi \sim 1 \). In Fig.(1.4) we show results for several \( \gamma \) fixing \( \xi = \pi \). For \( \gamma < 0.2 \) still a pronounced peak shows up at \( \omega \sim 0 \), on the other hand \( C(\omega) \) becomes for \( \gamma > 0.3 \) nearly constant or very slowly varying in a broad range of \( \omega/T \).

The main message of the above simple analysis is that for systems with overdamped QP excitations the universal form (1.5) describes quite well \( \sigma(\omega) \) for a wide range of parameters. It should be stressed that nearly constant \( C(\omega < \omega^*) \) also means that the current relaxation rate \( 1/\tau^* \) is very large, \( 1/\tau^* \sim \omega^* \gg 1/\tau \), i.e. much larger than the conductivity relaxation scale apparent from Eq.(1.5) where \( 1/\tau \propto T \) follows solely from thermodynamics.

One should also be aware of the upper cutoff scale \( \omega^* \) for the validity of the MFL-like QP damping. In the problem considered here it appears that the cutoff is directly related to the current relaxation rate \( \omega^* \sim 1/\tau^* \) found in the \( t-J \) model to be extremely high at the intermediate doping, i.e. \( \omega^* \sim 2t \). The latter allows for an effective mean free path \( l^* \) of only few cells, essentially independent of \( T \). Such a short \( l^* \) can be plausibly explained by assuming that charge carriers - holes entirely lose the phase coherence in collisions with each
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Figure 1.4 Current-current correlation spectra \(C(\omega)\) vs. \(\omega/T\) for various \(\gamma\) at fixed \(\xi = \pi\).

other due to the randomizing effect of an incoherent spin background. Note again that the short correlation length (even at \(T < T_c\)) appears also from the analysis of ARPES spectral functions \(A(k, \omega)\) varying \(\Delta k_{\parallel}\) along the Fermi surface [11].

4. DISCUSSION

Cuprates in their metallic phase are anomalous in several respects. One important conclusion at least for theoreticians is that most of anomalous properties are quite well reproduced also in the prototype \(t-J\) model. The analysis of this model has been so far restricted to numerical calculations of small systems, nevertheless in the \(T > T_{fs}\) window where macroscopic relevance of FTLM results is expected the agreement with experiments is even quantitative, without any adjustable parameters. Since the behaviour found experimentally is quite generic and universal down to lowest \(T \sim T_c\) there is no reason to doubt in the generality of model results.

Nevertheless there are open questions of the existence and the origin of low energy scales in cuprates as well as in the \(t-J\) model. In the underdoped or weakly doped regime FTLM shows the indication for the pseudogap scale \(T^*\), in particular in the uniform susceptibility \(\chi_0\) and in the density of states [4]. This scale seems to be related to the onset of short range AFM correlations, hence \(T^* \propto J\). Still for \(T < T^*\) the entropy remains large as manifested by experiments and our results. The electron liquid is thus closer to a nondegenerate system of composite particles than to a degenerate Fermi gas. Only at
$T \to 0$ the entropy is low enough to make the discussion of possible orderings or instabilities relevant.

The origin of the MFL behaviour of several dynamic quantities and of the universal form of $\sigma(\omega)$ and $\chi_L(\omega)$ in the intermediate doping has to be intimately related to the large degeneracy in this regime. It has been shown that QP are essentially overdamped down to lowest $T \sim T_c$. This can be only explained by the scattering on spin fluctuations, which mainly contribute to the entropy. On the other hand spins are just strongly perturbed by holes introduced by doping, so a self-consistent enhancement seems to be the mechanism which dominates the relevant physics. Only at low $T \sim T_c$ apparently this behaviour breaks down by an emergence of coherence and new energy scales.

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