Chapter 1

DIAMAGNETIC PROPERTIES OF DOPED ANTIFERROMAGNETS

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Abstract Finite-temperature diamagnetic properties of doped antiferromagnets as modeled by the two-dimensional t-J model were investigated by numerical studies of small model systems. Two numerical methods were used: the worldline quantum Monte Carlo method with a loop cluster algorithm (QMC) and the finite-temperature Lanczos method (FTLM), yielding consistent results. The diamagnetic susceptibility introduced by coupling of the magnetic field to the orbital current reveals an anomalous temperature dependence, changing character from diamagnetic to paramagnetic at intermediate temperatures.

The dc orbital susceptibility of the system in the external magnetic field is

$$\chi_d = -\mu_0 \frac{\partial^2 F}{\partial B^2} = -\frac{\chi_0}{\beta}\left[\frac{1}{Z}\frac{\partial^2 Z}{\partial \alpha^2} - \left(\frac{1}{Z}\frac{\partial Z}{\partial \alpha}\right)^2\right], \qquad (1.1)$$

where $\chi_0 = \mu_0 e^2 a^4/\hbar^2$ and $\alpha = eBa^2/\hbar$. In the previous studies [1] it was realized that results are quite sensitive to finite-size effects, so we also used the QMC method, where much larger lattices can be studied.

The magnetic field introduced into the t-J Hamiltonian via the Peierls construction, affects only the hopping of the electrons. Within FTLM the results are obtained by the numerical derivation with respect to α.

Using the standard Trotter-Suzuki decomposition and the *woldline* representation of the QMC for the fermionic models, magnetic field enters matrix elements concerning the hole hopping. The plaquette weights along the hole worldline obtain an additional phase factor. Taking the field derivatives explicitely the expresson for the orbital susceptibility can be written as

$$\chi_d = -\chi_0 \frac{\langle \mathcal{S}^2 \rangle}{\beta}, \qquad (1.2)$$

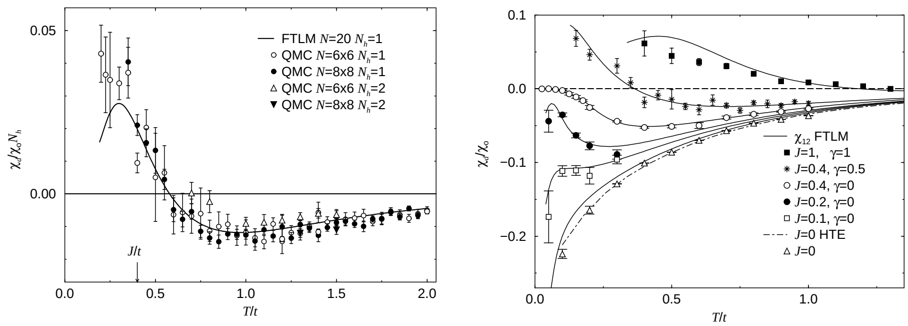

Figure 1.1 Orbital susceptibility χ_d vs. T (left) for one hole obtained via QMC (dots) and FTLM (line) for $J = 0.4t$; different J and γ (right). For comparison also results of high-temperature expansion (HTE) for $J = 0$ are shown (dash-dotted line).

where $\mathcal{S}$ is the projected area of the hole worldline. χ_d can be thus measured without the presence of a magnetic field. This is just another consequence of the more general fluctuation–dissipation theorem. In doped systems we are hindered by the well known "fermionic sign problem" of the QMC, not present in the undoped case. Even though $\mathcal{S}^2$ is strictly positive, the thermal average $\left\langle \mathcal{S}^2 \right\rangle$ can become negative because of correlations between the Monte Carlo sign and the magnitude of the area $\mathcal{S}$. For QMC the sizes of considered systems were 6×6 and 8×8.

With FTLM a few mobile holes on a system of tilted squares with up to 20 sites and periodic boundary conditions were considered. It is nontrivial to incorporate Landau phases corresponding to a homogeneous B, being at the same time compatible with periodic boundary conditions. This is possible only for quantized magnetic fields.

In Fig. 1.1, χ_d obtained via both methods is presented. For $T \gg t$, the response is diamagnetic and proportional to T^{-3} as well as essentially J-independent [1]. The most striking effect is that the orbital response below some temperature T_p turns from diamagnetic to paramagnetic, consistent with the preliminary results obtained via the FTLM [1]. In order to locate the origin of this phenomenon, results for different J and anisotropies γ are also shown. It appears that T_p scales with γJ, i.e. at $J = 0$ the response is clearly diamagnetic at all T, and for $\gamma = 0, J > 0$ no crossing is observed with either method.

At lower temperatures $T < T_d \ll T_p$, the diamagnetic behavior is expected to be restored. This follows from the argument that at $T \to 0$ a hole in an AFM should behave as a quasiparticle with a finite effective mass, exhibiting a cyclotron motion in $B \neq 0$, leading to $\chi_d(T \to 0) \to -\infty$ [1]. Numerically it is easiest to test this conjecture for a single hole and $\gamma = 0$. This is also true for $J = 0$.

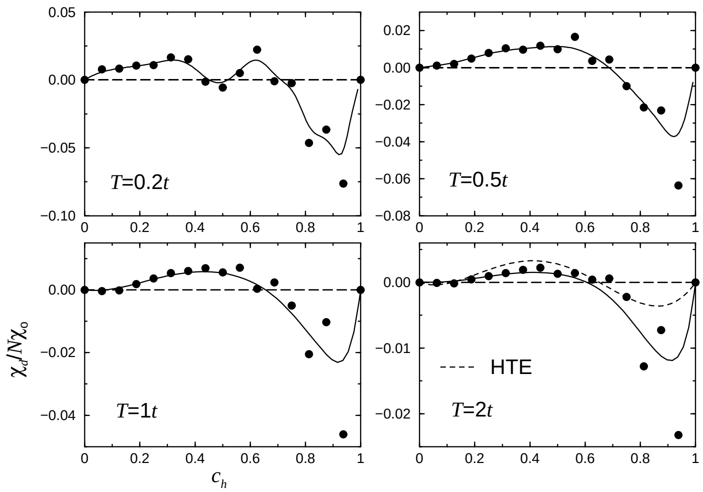

Figure 1.2 χ_d vs. c_h for several T and $J = 0.4t$. The last graph contains also a 4$^{\text{th}}$ order HTE result (dotted). Canonical (dots) and grand-canonical (line) values for all c_h are obtained with FTLM on 16 sites.

In Fig. 1.2 also results for χ_d for finite doping $c_h > 0$ are presented. For nearly empty band $c_h > 0.7$ the χ_d is diamagnetic and weakly dependent on T. In this dilute regime strong correlations are unimportant, thus Landau diamagnetism is expected. At moderate temperatures $T > J$ and for an intermediate-doping $0.2 < c_h < 0.7$ the χ_d is dominated by a paramagnetic response. There is a weak diamagnetism at $c_h < 0.2$ and $T > T_p$, while the paramagnetic regime extends to $c_h = 0$ for $T < T_p$. For low temperatures $T \ll J$ quite pronounced oscillations in $\chi_d(c_h)$ appear and can be partly attributed to finite-system effects.

The explanation can go in the direction proposed by [5], that at low doping $c_h \to 0$ we are dealing with quasiparticles (with a diamagnetic response), being a bound composite of charge (holon) and spin (spinon) elementary excitations. The binding appears to be quite weak and thus easily destroyed by finite T or c_h, enabling the independent and apparently paramagnetic response of constituents.

References

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