DYNAMICS OF CHARGE CARRIERS IN 2-D QUANTUM ANTIFERROMAGNETS

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Abstract. *We discuss the propagation of holes in the t-J model at low doping concentration using a formulation where the carriers are described by spinless fermions coupled to spin waves. The single-particle Green's function is evaluated numerically within self-consistent Born approximation which has been shown to agree quite well with spectra from exact diagonalization studies. We have shown that the spectral weight of the spin-polaron bound state scales with the inverse of the linear dimension. Based on this we find for the thermodynamic limit* $a_\infty = 0.62(J/t)^{0.72}$ *for values* $0.1 \leq J/t \leq 0.4$. *Furthermore we compare with the dominant pole approximation and determine its range of validity.*

The motion of spin-1/2 charge carriers in two-dimensional quantum Heisenberg antiferromagnets (AF) is intimately related to the dynamics of holes doped in copper-oxide-based superconductors. The problem of a single hole is relevant for the transition from the insulating AF phase to the metallic non-magnetic phase. The t-J model is used for this purpose:

$$H = -t \sum_{<ij>} (1-n_{i,-\sigma}) c_{i\sigma}^{+} c_{j\sigma} (1-n_{j,-\sigma}) + J \sum_{<ij>} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j \right) . \quad (1)$$

Treating the spin excitations in long-range AF linear spin-wave theory and using a holon representation [1-3], the kinetic energy of the t-J model transforms into the coupling term to spin waves. Thus the problem is very similar to the Fröhlich polaron model. An essential difference is the absence of a free kinetic energy for the holons. The resulting spin-polaron propagates on the scale of J, which is merely a consequence of the coupling to the AF spin excitations, unlike the conventional (*charge*-)polaron solution. Although the physical parameters are $t > J$, we use a self-consistent expansion of second order in t [1,2] which amounts to a summation of the non-crossing diagrams. In this Born approximation the hole propagator thus obeys the integral equation

$$G(\mathbf{k},\omega) = \frac{1}{\omega - \sum_{\mathbf{q}} M^2(\mathbf{k},\mathbf{q})\, G(\mathbf{k}-\mathbf{q},\omega-\omega_{\mathbf{q}})} \; ; \qquad M(\mathbf{k},\mathbf{q}) = \frac{zt}{\sqrt{N}} \left| u_{\mathbf{q}} \gamma_{\mathbf{k}-\mathbf{q}} + v_{\mathbf{q}} \gamma_{\mathbf{k}} \right| , \quad (2)$$

where $M(\mathbf{k},\mathbf{q})$ represents the coupling of the hole at wavevector $\mathbf{k}$ to spin excitations of wavevectors $\mathbf{q}$, with energies $\omega_{\mathbf{q}}$, and is depicted in Fig. 1-a for $\mathbf{k} = (\pi/2, \pi/2)$: the bottom of the qp band. For long wavelengths $q \sim 0$ the coupling to magnons has dipolar character, $M \propto (\nabla\gamma_{\mathbf{k}})\cdot\mathbf{q}/q^{1/2}$, like in McMillan's theory of liquid ^{3}He —^{4}He dilute mixtures [see also Ref. 4], and it is zero for $\mathbf{q} = 0$ and (π, π). Thus the coupling to short wavelengths alone is important.

We have recently shown [3] by numerical solution of this integral equation that the resulting spectral functions $A(\mathbf{k},\omega)$ are in detailed agreement with exact diagonalization studies [5]. These spectra, like the one in Fig. 1-b, show a bound state due to the formation of an antiferromagnetic spin-polaron [3], which has a dispersion of order J with a minimum at $(\pi/2, \pi/2)$ and a maximum at the Γ-point. So the quasiparticle Fermi surface is pocket-like with four degenerate valleys. Further an incoherent

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background, due to multiple-spin excitations, of width $\leq 7t$ is formed above the spin-polaron and it may explain [6] the anomalous mid-infrared absorption in the conductivity experiments of these compounds.

Our quantitative analysis has shown that in 2-D the residue of the quasiparticle at $(\pi/2, \pi/2)$ obeys the scaling law [3] $a(L) = a_\infty + b/L$, with L the linear dimension, $N = L \times L$. We note that this result is not limited to the perturbative case. For values $J/t = 0.1, 0.2, 0.3, 0.4$ the following results are obtained $a_\infty = 0.114, 0.198, 0.262, 0.317$ and $b = 0.267, 0.327, 0.355, 0.386$ respectively, where a_∞ is the spectral weight in the thermodynamic limit, and it can be fitted by $a_\infty \sim 0.62(J/t)^{0.72}$.

In the dominant pole approximation [2] $G(\mathbf{k}, \omega) \sim a_\mathbf{k}/(\omega - \varepsilon_\mathbf{k})$, where the incoherent background is ignored, the residue and positions of the quasiparticle can be self-consistently obtained from

$$a_\mathbf{k} = \left[1 + \sum_\mathbf{q} \frac{M^2(\mathbf{k},\mathbf{q})\, a_{\mathbf{k}-\mathbf{q}}}{(\varepsilon_\mathbf{k} - \varepsilon_{\mathbf{k}-\mathbf{q}} - \omega_\mathbf{q})^2}\right]^{-1} ; \qquad \varepsilon_\mathbf{k} = \Sigma(\mathbf{k}, \varepsilon_\mathbf{k}) = \sum_\mathbf{q} \frac{M^2(\mathbf{k},\mathbf{q})\, a_{\mathbf{k}-\mathbf{q}}}{\omega - \omega_\mathbf{q} - \varepsilon_{\mathbf{k}-\mathbf{q}} + i\delta}\bigg|_{\omega=\varepsilon_\mathbf{k}} . \qquad (3)$$

Figure 1-c shows the comparison of our results with the latter approximation for a 16×16 cluster. We observe that $\varepsilon_\mathbf{k}$ differs already for $J = t$ by 15% whereas the deviations in $a_\mathbf{k}$ are small, since Eq. (3) forces $a_\mathbf{k} \to 0$ for $J \to 0$. Hence the use of the dominant pole approximation for *quantitative* purposes is restricted to the intermediate and weak coupling limits $J \geq t$. On the other hand, the full solution of Eq. (2) is a reliable approach for the description of a few holes in a quantum antiferromagnet for any coupling strength [3], as it produces results which are in close agreement with the exact diagonalization studies even in the strong-coupling regime.

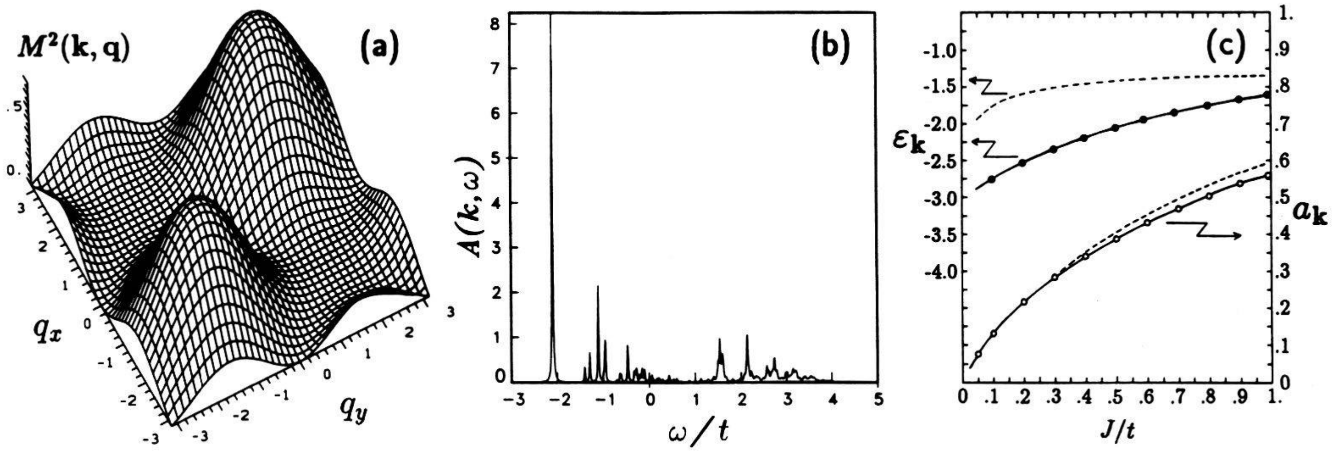

Fig. 1 (a) Matrix elements in Eq. (2) at $\mathbf{k} = (\pi/2, \pi/2)$ showing the coupling 'across the valleys'.
(b) Spectral function of the spin-polaron for $J/t = 0.2$ at $\mathbf{k} = (\pi/2, \pi/2)$ in a 4×4 cluster.
(c) Comparison of the dominant pole (dashed-lines) and Born (solid-lines) approximations.

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