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## 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:

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

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

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

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  $^3\text{He} - ^4\text{He}$  dilute mixtures [see also Ref. 4], and it is zero for  $\mathbf{q} = 0$  and  $(\pi, \pi)$ . 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  $\Gamma$ -point. So the quasiparticle Fermi surface is pocket-like with four degenerate valleys. Further an incoherent

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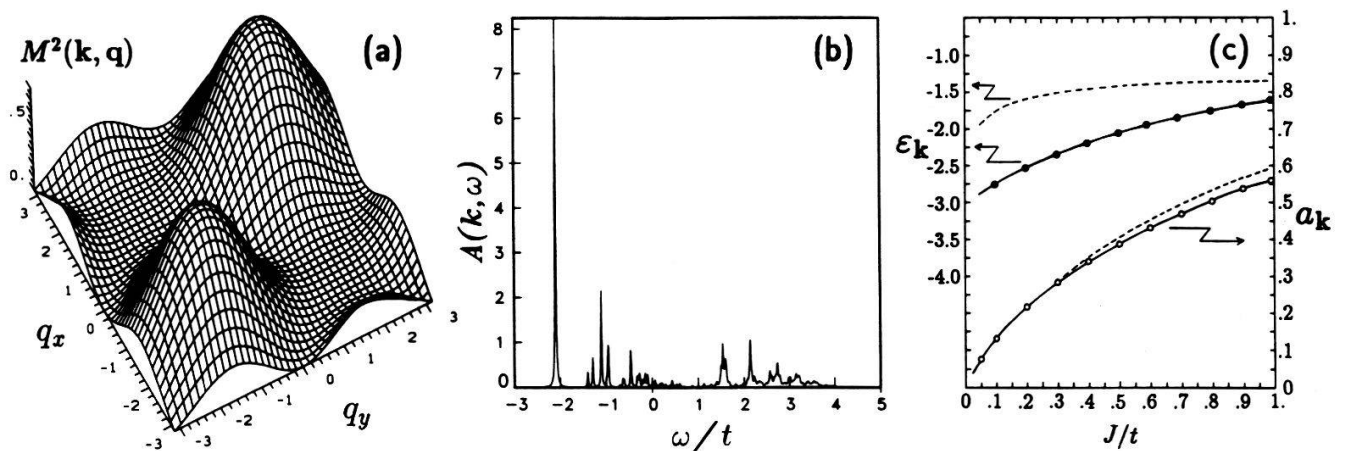
background, due to multiple-spin excitations, of width  $\leq 7t$  is formed above the spin-polaron and it may explain [6] the anomalous mid-infrared absorption in the conductivity experiments of these compounds.

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  $a_\infty$  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

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

Figure 1-c shows the comparison of our results with the latter approximation for a  $16 \times 16$  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  $a_{\mathbf{k}} \rightarrow 0$  for  $J \rightarrow 0$ . 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  $4 \times 4$  cluster. (c) Comparison of the dominant pole (dashed-lines) and Born (solid-lines) approximations.

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