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Autor: Martínez, Gerardo / Horsch, Peter
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DYNAMICS OF CHARGE CARRIERS IN 2-D QUANTUM ANTIFERROMAGNETS

Gerardo Martínez ^{a,1} and Peter Horsch ^b^aInstituto de Física, UNICAMP, 13100 Campinas, SP, Brasil^bMax-Planck-Institut für Festkörperforschung, 7000 Stuttgart 80, Germany

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:

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

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 (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

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

Figure 1-c shows the comparison of our results with the latter approximation for a 16×16 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.

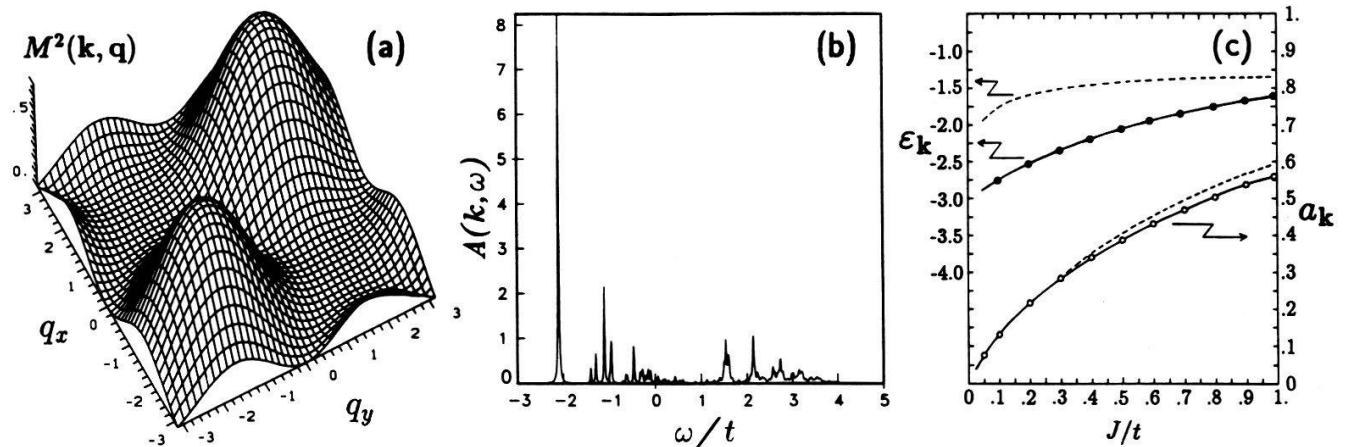


Fig. 1 (a) Matrix elements in Eq. (2) at $\mathbf{k} = (\pi/2, \pi/2)$ showing the coupling ‘across the valleys’.
(b) Spectral function of the spin-polaron for $J/t = 0.2$ at $\mathbf{k} = (\pi/2, \pi/2)$ in a 4×4 cluster.
(c) Comparison of the dominant pole (dashed-lines) and Born (solid-lines) approximations.

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