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Wave function and size of spin-polarons in the t-J model

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Here we present a more detailed picture of some spatial properties of the spin-polaron - quasiparticle formed after injecting a hole into a planar quantum antiferromagnet. The explicit form of the quasiparticle wave function allows us accurately to investigate the spatial extent of the polaron. In the Ising limit of the model we find for the RMS radius of the distribution of spin-deviations around the moving hole is $R = 1.06(t/J)^{0.157}$. The form and the size of the polaron in the usual t-J model (Heisenberg limit), is on the other hand, anisotropic, larger and does not obey such a simple scaling. Finally we discuss the renormalization of spin-polarons by phonons in the framework of a Holstein t-J model.

The problem of a single mobile vacancy (hole) in an antiferromagnetic (AFM) plane was extensively investigated using various analytical approaches as well as with exact diagonalization of small clusters[1]. In this work we present a more detailed picture of the quasiparticle, in paricular the spatial size of spin-polaron.

We study the t-J Hamiltonian reformulated in terms of spinless fermions and Schwinger bosons [2]. We first calculate the Green's function for the hole in self-consistent Born approximation from the equation $\Sigma_{\mathbf{k}}(\omega) = \frac{1}{N}\sum_{\mathbf{q}} M^2_{\mathbf{kq}} G_{\omega-\mathbf{q}}(\omega-\omega_{\mathbf{q}})$ for the self-energy, where $M_{\mathbf{kq}}$ is the fermion-magnon coupling and $\omega_{\mathbf{q}}$ is magnon dispersion. The corresponding wave function [3,4] is given by

$$\begin{aligned}|\Psi_{\mathbf{k}}\rangle &= Z_{\mathbf{k}}^{1/2}\Big[\, h^\dagger_{\mathbf{k}} + N^{-1/2}\sum_{\mathbf{q}_1} g_{\mathbf{k},\mathbf{q}_1} h^\dagger_{\mathbf{k}_1}\alpha^\dagger_{\mathbf{q}_1} + \cdots \\ &\quad + N^{-n/2}\sum_{\mathbf{q}_1,\ldots,\mathbf{q}_n} g_{\mathbf{k},\mathbf{q}_1} g_{\mathbf{k}-\mathbf{q}_1,\mathbf{q}_2}\cdots \\ &\quad \times g_{\mathbf{k}-\mathbf{q}_1-\ldots-\mathbf{q}_{n-1},\mathbf{q}_n} h^\dagger_{\mathbf{k}-\mathbf{q}_1-\ldots-\mathbf{q}_n} \\ &\quad \times \alpha^\dagger_{\mathbf{q}_1}\cdots\alpha^\dagger_{\mathbf{q}_n}\Big]|AFM\rangle. \qquad (1)\end{aligned}$$

Here $h^\dagger_{\mathbf{k}}$ is the creation operator for a hole and $\alpha^\dagger_{\mathbf{q}}$ creates an AFM magnon. The coefficients $g_{\mathbf{k},\mathbf{q}}$ are determined with the Green's function and $g_{\mathbf{k},\mathbf{q}} = M_{\mathbf{kq}} G_{\mathbf{k}-\mathbf{q}}(\omega - \omega_{\mathbf{q}})$. The Green's function is evaluated at the energy of the quasiparticle pole, $\omega = \epsilon_{\mathbf{k}}$. The normalization constant is derived from the self-energy, $Z^{-1}_{\mathbf{k}} = 1 - \partial\Sigma_{\mathbf{k}}(\omega)/\partial\omega|_{\epsilon_{\mathbf{k}}}$. The state $|AFM\rangle$ represents the vacuum with respect to hole and magnon operators.

The wave-function can be used to extract various correlation functions. First we calculate the average number of magnons excited by the hole, $< n >= \langle\Psi_{\mathbf{k}}|\sum_{\mathbf{q}}\alpha^\dagger_{\mathbf{q}}\alpha_{\mathbf{q}}|\Psi_{\mathbf{k}}\rangle$. In the Ising limit of the model (transverse coupling in the t-J Hamiltonian set to zero) $< n >$ is identical to the average number of local spin deviations, $\langle\sum_i S^+_i S^-_i\rangle$, and is proportional to the average string length l_{av} in the corresponding confining linear string potential. Therefore $< n > \propto l_{av} \propto (t/J)^{1/3}$ for $J/t \ll 1$ as presented in [5]. The same scaling is expected for the *spatial size* of the polaron.

A measure of the the spatial extent of the polaron is given by the correlation function

$$N_{\mathbf{R}} = \langle\Psi_{\mathbf{k}}|\sum_i n_i a^\dagger_{i+\mathbf{R}} a_{i+\mathbf{R}}|\Psi_{\mathbf{k}}\rangle,$$

where $n_i = h^\dagger_i h_i$ is density operator for holes. This correlation function measures the average number of (local) magnons excited at the distance $\mathbf{R}$ from the hole. The counting of bosons with $a^\dagger_i a_i$ on the level of Holstein-Primakoff approximation used in our treatment corresponds to the counting of spin deviations, $S^+_i S^-_i$. The function $N_{\mathbf{R}}$ can be used to determine the size of the polaron.

In the Ising limit $N_{\mathbf{R}}$ can be decomposed into $N_{\mathbf{R}} = \sum_{m=1}^{\infty} p_m(\mathbf{R}) P_m$, where $P_m = \sum_{j=m}^{\infty} A^{(j)}$

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and $p_m(\mathbf{R}) = 4^{-m}\binom{m}{m_+}\binom{m}{m_-}$. Here $m_\pm = \frac{1}{2}(m - ||R_x| \pm |R_y||)$ must be a non-negative integer, otherwise $p_m(\mathbf{R}) = 0$. $A^{(n)}$ is the probability distribution that n magnons are excited and is given with the recursion relation, $A^{(m+1)} = A^{(m)}[2tG_{\mathbf{k}}(\epsilon_{\mathbf{k}} - 2mJ)]^2$ and $A^{(0)} = Z_{\mathbf{k}}$. In the Ising limit there is no momentum dependence of the quasiparticle.

We define the size of the polaron quantitatively by the radius R_p (element of Bravais lattice), which encloses a given fraction p of the total number of spin deviations, $p =< n >^{-1} \sum_{R \le R_p} N_{\mathbf{R}}$. In the Fig. 1 we present R_p vs. J/t for three different values of p = 0.7, 0.9, and 0.99. In the physically interesting regime, $J/t \sim 0.3$ the polaron is contained within the radius < 2. The expected scaling $R_p \propto < n >^{1/2} \propto (t/J)^{1/6}$ is well established. We have also calculated the average radius, $R_{ave} =< n >^{-1} \sum_{\mathbf{R}} |\mathbf{R}| N_{\mathbf{R}}$, and the root-mean square radius, R_{RMS}. In Fig. 1 R_{RMS} and R_{ave} are presented with solid line and dashed line respectively. The RMS radius can be for $J/t < 1$ well fitted with $R = 1.06(t/J)^{0.157}$.

The form and the size of the polaron in the usual t-J model (Heisenberg limit), is on the other hand, anisotropic, much larger and does not obey such a simple scaling. The average radius cannot be defined, because of a slow power-law $\sim 1/R^2$ dependence of $N_{\mathbf{R}}$ for $R \to \infty$ and thus logarithmically divergent $< n >$ [4].

Finally, we have studied also the renormalization of spin-polarons by phonons in the framework of a Holstein t-J model,

$$H = H_{tJ} + \sum_{i\delta s} M_\delta c_{is}^\dagger c_{is}(b_{i+\delta}^\dagger + b_{i+\delta}) + \Omega \sum_i b_i^\dagger b_i,$$

where H_{tJ} is the usual t-J Hamiltonian with coupling of charge carriers to Einstein phonons with energy Ω and the fermion-phonon coupling M_δ [6]. We found that the slow coherent motion of the polaron enhances the effect of the lattice distortion. The phonon induced mass renormalization of the carriers which propagate in the t-J model on scale J is much larger than in the corresponding uncorrelated model, except in the limit of $J \to 0$ where the weight of the quasiparticle pole tends to zero. The enhancement is a consequence of the slow coherent motion of the spin polarons which makes electron-phonon interactions more effective. The corresponding wave function has the same structure as in the bare t-J model.

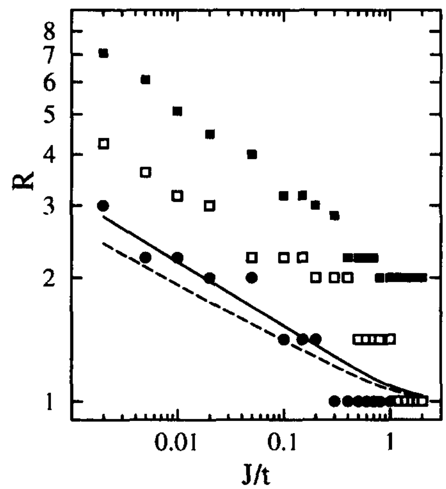

Figure 1. The radius R of a spin-polaron calculated with different definitions for R: R_p vs. J/t for three different values of p = 0.7 (circles), 0.9 (open squares) and 0.99 (full squares); R_{RMS} and R_{ave} are presented with solid line and dashed line respectively.

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