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Electron momentum distribution of a single mobile hole in the t-J model

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We investigate the electron momentum distribution function (EMDF) for the two-dimensional t-J model. The results are based on the self-consistent Born approximation (SCBA) for the self-energy and the wave function. In the Ising limit of the model we give the results in a closed form, in the Heisenberg limit the results are obtained numerically. An anomalous momentum dependence of EMDF is found and the anomaly is in the lowest order in number of magnons expressed analitycally. We interpret the anomaly as a fingerprint of an emerging large Fermi surface coexisting with hole pockets.

The electron momentum distribution function $n_{\mathbf{k}} = \langle \Psi_{\mathbf{k}_0} | \sum_\sigma c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} | \Psi_{\mathbf{k}_0} \rangle$ is the key quantity for resolving the structure of the Fermi surface in cuprates [1]. Here we study the EMDF for $|\Psi_{\mathbf{k}_0}\rangle$ which represents a weakly doped antiferromagnet (AFM), i.e., it is the ground state (GS) wave function of a planar AFM with one hole and with the total momentum $\mathbf{k}_0$. In the present work we investigate the low-energy physics of the CuO_2 planes in cuprates within the framework of the standard t-J model

$$\begin{aligned} H &= -t \sum_{<ij>\sigma} (\tilde{c}^\dagger_{i,\sigma} \tilde{c}_{j,\sigma} + \mathrm{H.c.}) + \\ &\quad + J \sum_{<ij>} [S^z_i S^z_j + \frac{\gamma}{2}(S^+_i S^-_j + S^-_i S^+_j)], \quad (1) \end{aligned}$$

where $\tilde{c}^\dagger_{i,\sigma}$ ($\tilde{c}_{i,\sigma}$) are electron creation (annihilation) operators acting in a space forbidding double occupancy on the same site. S^α_i are spin operators. Our approach is based on a spinless fermion Schwinger boson representation of the t-J Hamiltonian [2] and on the SCBA for calculating the Green's function $G_{\mathbf{k}}(\omega)$ [2-4] and the corresponding wave function $|\Psi_{\mathbf{k}}\rangle$ [5].

In general the expectation value $n_{\mathbf{k}}$ has to be calculated numerically. The Ising limit, $\gamma = 0$, is an exception. The quasi particle is dispersionless with the GS energy $\epsilon_{\mathbf{k}} = \epsilon_0$, the residue $Z_{\mathbf{k}} = Z_0$ and the Green's function $G_{\mathbf{k}}(\omega) = G_0(\omega)$. Therefore it is possible to express the required matrix elements in $n_{\mathbf{k}}$ analytically and to perform a summation of corresponding non-crossing contributions to any order $n \to \infty$. The result is

$$\begin{aligned} n_{\mathbf{k}} &= 1 - \frac{1}{2} Z_0 (\delta_{\mathbf{k}\mathbf{k}_0} + \delta_{\mathbf{k}\mathbf{k}_0+\mathbf{Q}}) + \frac{1}{N}\delta n_{\mathbf{k}}, \quad (2) \\ \delta n_{\mathbf{k}} &= 4P\gamma_{\mathbf{k}} - 4(1-Z_0)\gamma^2_{\mathbf{k}}, \quad (3) \end{aligned}$$

where $P = \sum_{m=0}^\infty \sqrt{A_m A_{m+1}}$ with $A_0 = Z_0$, $A_m = A_{m-1}[2tG_0(\epsilon_0 - 2mJ)]^2$, $\sum_{m=0}^\infty A_m = 1$ [5] and $\gamma_{\mathbf{k}} = (\cos k_x + \cos k_y)/2$. We note that the result Eqs. (2,3) exactly fulfills the sum rule $\sum_{\mathbf{k}} n_{\mathbf{k}} = N - 1$ and $\delta n_{\mathbf{k}} \le 1$. In Eq. (2) the only dependence on the GS momentum $\mathbf{k}_0$ enters through the two delta functions separated with the AFM vector $\mathbf{Q} = (\pi, \pi)$. The EMDF $\delta n_{\mathbf{k}}$ is determined only with two parameters, P and Z_0, presented as a function of J/t in Fig. 1. Note that $P = 1$ and $Z_0 = 0$ for $J \to 0$, therefore the result simplifies, $\delta n_{\mathbf{k}} = 4\gamma_{\mathbf{k}}(1 - \gamma_{\mathbf{k}})$.

Now we turn to the Heisenberg model, $\gamma \to 1$. Here the important ingredient is the gap-less magnons with linear dispersion and a more complex ground state of the planar AFM. $G_{\mathbf{k}}(\omega)$ is strongly $\mathbf{k}$-dependent. The GS is fourfold degenerate and the results must be averaged over the GS momenta $\mathbf{k}_0 = (\pm\pi/2, \pm\pi/2)$. To get more insight into the structure of $\delta n_{\mathbf{k}}$, we simplify the wave function by keeping only the one-magnon contributions. The leading order contribution to

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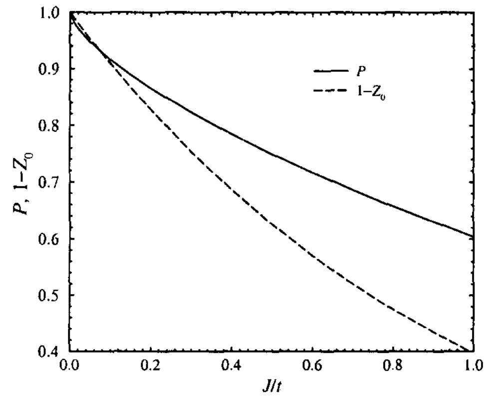

Figure 1. $P = \sum_{m=0}^{\infty} \sqrt{A_m A_{m+1}}$, full line, and $1 - Z_0$, dashed line, determine all momentum dependence of $\delta n_{\mathbf{k}}$ in the SCBA with $\gamma = 0$.

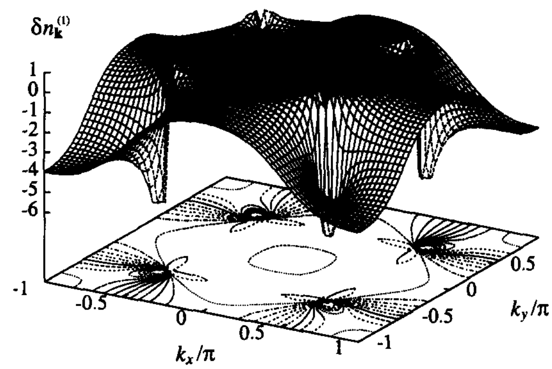

Figure 2. Perturbative result $\delta n_{\mathbf{k}}^{(1)}$, Eq. (4), for $Z_{\mathbf{k}} t/J \sim 1$.

$\delta n_{\mathbf{k}}$ is then

$$\begin{aligned}\delta n_{\mathbf{k}}^{(1)} &= -Z_{\mathbf{k}_0} M_{\mathbf{k}_0\mathbf{q}} G_{\mathbf{k}_0}(\epsilon_{\mathbf{k}_0} - \omega_{\mathbf{q}}) \times \\ &\quad \times \left[2u_{\mathbf{q}} + M_{\mathbf{k}_0\mathbf{q}} G_{\mathbf{k}_0}(\epsilon_{\mathbf{k}_0} - \omega_{\mathbf{q}})\right], \qquad (4)\end{aligned}$$

with $\mathbf{q} = \mathbf{k} - \mathbf{k}_0$ [or equivalent in the Brillouin zone (BZ)], $\mathbf{v} = t(\sin k_{0x}, \sin k_{0y})$ and $M_{\mathbf{k}_0\mathbf{q}}$ is the hole-magnon coupling [2,3]. The momentum dependence of the EMDF, contained in Eq. (4), essentially captures well the full numerical solution [6]. A surprising observation is that the EMDF exhibits in the extreme Heisenberg limit a discontinuity $\sim Z_{\mathbf{k}_0} N^{1/2}$ and $\delta n_{\mathbf{k}}^{(1)} \propto -(1 + \operatorname{sign} q_x)/q_x$. We interpret this result as an indication of an emerging *large* Fermi surface at discontinuities at *points* $\mathbf{k}_0$, *not lines* in the BZ. The anomalous structure at $\mathbf{k} = (\pm\pi/2, \pm\pi/2)$ is clearly seen in Fig. 2, where $\delta n_{\mathbf{k}}^{(1)}$ is shown for $Z_{\mathbf{k}} t/J \sim 1$ and $\gamma \to 1$. The Green's function is here approximated with the non-interacting expression, $G_{\mathbf{k}_0}(\omega) \approx -1/\omega$. It should be noted that $\delta n_{\mathbf{k}}^{(1)}$ exhibits at $\gamma = 1$ also a (weak) singularity (> 1). However, the $n_{\mathbf{k}}$ sum rule is still exactly satisfied. In Fig. 2 is for the purpose of presentation $\delta n_{\mathbf{k}}^{(1)}$ truncated to $-6 < \delta n_{\mathbf{k}}^{(1)} < 1$.

In the present work we considered the electron momentum distribution function for a single hole in AFM and possibly relevant to underdoped cuprates. Non-analytic properties encountered in Eq. (4) are an evidence of the emerging *large* Fermi surface at $\mathbf{k} \sim (\pm\pi/2, \pm\pi/2)$ coexisting, however, with a 'hole pocket' type of a Fermi surface. As long-range AFM order is destroyed by doping, 'hole-pocket' contributions should disappear while the singularity in $\delta n_{\mathbf{k}}$ could persist. We thus interpret this result as relevant for the understanding of the electronic structure found recently with ARPES experiments in uderdoped cuprates [1], where only portions of a large Fermi surface close to $\mathbf{k} \sim \mathbf{k}_0$ were seen.

REFERENCES

1. Z.-X. Shen and D. S. Dessau, Phys. Rep. **253**, 1 (1995); B. O. Wells *et al.*, Phys. Rev. Lett. **74**, 964 (1995); D. S. Marshall *et al.*, Phys. Rev. Lett. **76**, 4841 (1996).
2. S. Schmitt-Rink *et al.*, Phys. Rev. Lett. **60**, 2793 (1988).
3. A. Ramšak and P. Prelovšek, Phys. Rev. B **42**, 10415 (1990).
4. G. Martínez and P. Horsch, Phys. Rev. B **44**, 317 (1991).
5. A. Ramšak and P. Horsch, Phys. Rev. B **48**, 10559 (1993); *ibid.* **57**, 4308 (1998).
6. A. Ramšak, I. Sega, and P. Prelovšek, cond-mat/9910419.