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 analytically. We interpret the anomaly as a fingerprint of an emerging large Fermi surface coexisting with hole pockets.

The electron momentum distribution function \( n_k = \langle \Psi_{k0} | \sum_{\sigma} c_{k,\sigma}^\dagger c_{k,\sigma} | \Psi_{k0} \rangle \) is the key quantity for resolving the structure of the Fermi surface in cuprates [1]. Here we study the EMDF for \( |\Psi_{k0}\rangle \) 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 \( k_0 \). 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

\[
H = -t \sum_{<ij>\sigma} (\tilde{c}_{i,\sigma}^\dagger \tilde{c}_{j,\sigma} + \text{H.c.}) + J \sum_{<ij>} \left[ \vec{S}_i \cdot \vec{S}_j + \frac{\gamma}{2} (\vec{S}_i^+ \vec{S}_j^- + \vec{S}_i^- \vec{S}_j^+) \right],
\]

(1)

where \( \tilde{c}_{i,\sigma}^\dagger (\tilde{c}_{i,\sigma}) \) are electron creation (annihilation) operators acting in a space forbidding double occupancy on the same site. \( \vec{S}_i \) 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 \( G_k(\omega) \) [2–4] and the corresponding wave function \( |\Psi_k\rangle \) [5].

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

\[
n_k = 1 - \frac{1}{2} Z_0 (\delta_{kk_0} + \delta_{kk_0+Q}) + \frac{1}{N} \delta n_k,
\]

(2)

\[
\delta n_k = 4P \gamma_k - 4(1 - Z_0) \gamma_k^2,
\]

(3)

where \( P = \sum_{m=0}^\infty \sqrt{A_m A_{m+1}} \) with \( A_0 = Z_0, A_m = A_{m-1}[2tG_0(\epsilon_0 - 2mJ)]^2, \sum_{m=0}^\infty A_m = 1 \) [3] and \( \gamma_k = (\cos k_x + ...
\[
cos k_y)/2. \text{ We note that the result Eqs. (2,3) exactly fulfills the sum rule } \sum_k n_k = N - 1 \text{ and } \delta n_k \leq 1. \text{ In Eq. (2) the only dependence on the GS momentum } k_0 \text{ enters through the two delta functions separated with the AFM vector } Q = (\pi, \pi). \text{ The EMDF } \delta n_k \text{ is determined only with two parameters, } P \text{ and } Z_0, \text{ presented as a function of } J/t \text{ in Fig. 1. Note that } P = 1 \text{ and } Z_0 = 0 \text{ for } J \rightarrow 0, \text{ therefore the result simplifies, } \delta n_k = 4\gamma_k(1 - \gamma_k). \]

Now we turn to the Heisenberg model, \( \gamma \rightarrow 1 \). Here the important ingredient is the gap-less magnons with linear dispersion and a more complex ground state of the planar AFM. \( G_k(\omega) \) is strongly \( k \)-dependent. The GS is fourfold degenerate and the results must be averaged over the GS momenta \( k_0 = (\pm \pi/2, \pm \pi/2) \). To get more insight into the structure of \( \delta n_k \), we simplify the wave function by keeping only the one-magnon contributions. The leading order contribution to \( \delta n_k \) is then

\[
\delta n_k^{(1)} = -Z_{k_0} M_{k_0,q} G_{k_0}(\epsilon_{k_0} - \omega_q) \left[ 2u_q + M_{k_0,q} G_{k_0}(\epsilon_{k_0} - \omega_q) \right], \tag{4}
\]

with \( q = k - k_0 \) [or equivalent in the Brillouin zone (BZ)], \( v = t(\sin k_{0x}, \sin k_{0y}) \), \( M_{k_0,q} \) is the hole-magnon coupling and \( u_q \) is the usual spin wave Bogoliubov coefficient [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 \( \sim Z_{k_0} N^{1/2} \) and \( \delta n_k^{(1)} \propto -(1 + \text{sign } q_x)/q_x \). We interpret this result as an indication of an emerging large Fermi surface at discontinuities at points \( k_0 \), not lines in the BZ.

The anomalous structure at \( k = (\pm \pi/2, \pm \pi/2) \) is clearly seen in Fig. 2, where \( \delta n_k^{(1)} \) is shown for \( Z_{k_0} t/J \sim 1 \) and \( \gamma \rightarrow 1 \). The Green’s function is here approximated with the non-interacting expression, \( G_{k_0}(\omega) \approx -1/\omega \). It should be noted that \( \delta n_k^{(1)} \) exhibits at \( \gamma = 1 \) also a (weak) singularity (> 1). However, the \( n_k \) sum rule is still exactly satisfied. In Fig. 2 is for the purpose of presentation \( \delta n_k^{(1)} \) truncated to \(-6 < \delta n_k^{(1)} < 1\).

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 \( k \sim (\pm \pi/2, \pm \pi/2) \) 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 \( \delta n_k \) could persist. We thus interpret this result as relevant for the understanding of the electronic structure found recently with ARPES experiments in underdoped cuprates [1], where only portions of a large Fermi surface close to \( k \sim k_0 \) were seen.
FIG. 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 \( \delta n_k \) in the SCBA with \( \gamma = 0 \).

FIG. 2. Perturbative result \( \delta n_k^{(1)} \), Eq. (4), for \( Z_k t/J \sim 1 \).

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