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# Electron momentum distribution function in the $t$–$t'$–$J$ model

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**Abstract**

We study the electron momentum distribution function (EMDF) for the two-dimensional $t$–$t'$–$J$ model doped with one hole on finite clusters by the method of twisted boundary conditions. The results quantitatively agree with our analytical results for a single hole in the antiferromagnetic background, based on the self-consistent Born approximation (SCBA). Moreover, within the SCBA an anomalous momentum dependence of EMDF is found, pointing to an emerging large Fermi surface. The analysis shows that the presence of next-nearest-neighbor (NNN) hopping terms changes EMDF only quantitatively if the ground state (GS) momentum is at (π/2,π2) and qualitatively if the GS momentum is shifted to (π,0). 

*Keywords:* Electron momentum distribution; Fermi surface; $t$–$J$ model

The existence and the character of the Fermi surface (FS) of high $T_c$ superconductors, in particular in their underdoped regime, is one of the open questions [1] of solid-state physics. The key quantity for resolving this problem is the electron momentum distribution function $n_k = \langle \Psi_{k_0} | \sum_\sigma c^\dagger_{k,\sigma} c_{k,\sigma} | \Psi_{k_0} \rangle$. Here we study the EMDF for $|\Psi_{k_0}\rangle$ which represents a weakly doped antiferromagnet (AFM), i.e., it is the GS wave function of a planar AFM with *one hole* and the GS wave vector $\boldsymbol{k}_0$. The wave function is determined within the framework of the standard $t$–$J$ model with nearest-neighbor hopping $t_{jj'} \equiv t$ and the AFM exchange is fixed to $J = 0.3t$. In order to come closer to the realistic situation in cuprates the model is extended with the NNN hopping $t_{jj'} \equiv t'$ for $jj'$ representing next-nearest-neighbors,

$$H = -\sum_{\langle jj' \rangle \sigma} t_{jj'} (\tilde{c}^\dagger_{j,\sigma} \tilde{c}_{j',\sigma} + \text{h.c.}) + J \sum_{\langle ij \rangle} \left[ S^z_i S^z_j + \frac{\gamma}{2} (S^+_i S^-_j + S^-_i S^+_j) \right]. \quad (1)$$

Numerically $n_k$ can be determined by exact diagonalization (ED) of the model Eq. (1) in small clusters, where only a restricted number of momenta $\boldsymbol{k}$ is allowed. The GS wave vector due to finite size effects varies with $N$. Therefore, we present here results obtained with the method of twisted boundary conditions [2], where $t_{jj'} \to t_{jj'} \exp(\mathrm{i}\theta_{jj'})$. Since, $n_k \equiv n_k(\boldsymbol{k}_0, \theta)$ depends both on $\boldsymbol{k}_0$ and $\theta$ it follows from Peierls construction that $n_k(\boldsymbol{k}_0, 0) = n_{k+k_0}(0, \boldsymbol{k}_0)$ for $\theta = \boldsymbol{k}_0$. This allows us to study $n_k$ for arbitrary $\boldsymbol{k}$ and $\boldsymbol{k}_0$. Furthermore, the finite size effects of the results are suppressed if we fix $\boldsymbol{k}_0$ for *all clusters* here studied to the symmetry point $\boldsymbol{k}_0 = (\pi/2, \pi/2)$.

In Fig. 1(a) we present ED results for clusters with different $N$ and $\gamma = 1$. The EMDF obeys the sum rule $\sum_k \boldsymbol{n}_k = N - 1$ and, for the allowed momenta, the constraint $N(n_k - 1) \leqslant 1$. We show here the quantity $N(n_k - 1)$, which for different $N$ scales towards the same curve. Results are presented for momenta $\boldsymbol{k} \in [(-\pi, -\pi) \to (\pi, \pi)]$ and should be averaged over all four possible ground state momenta when discussed, e.g., in connection with ARPES data.

We further compare the results with the self-consistent Born approximation [4], where we decouple fermion operators into hole and magnon operators [5–7], and using the SCBA wave function [6–8] we evaluate the required matrix elements in $n_k$. In Fig. 1(a) the result for $N(n_k - 1)$ is presented. In the SCBA there appear in $n_k$ at $\boldsymbol{k} \sim \boldsymbol{k}_0, \boldsymbol{k}_0 + (\pi, \pi)$ also delta-function contributions

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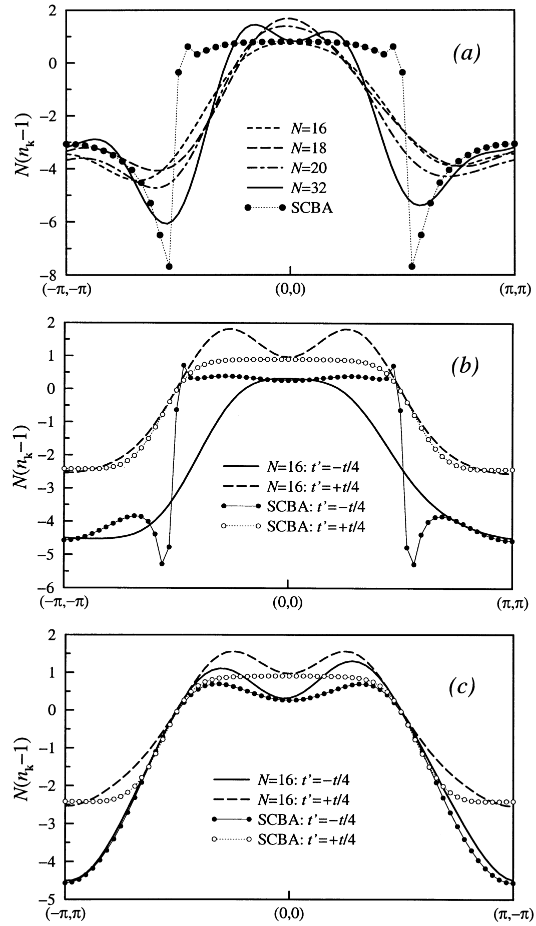


Fig. 1. $N(n_k - 1)$ obtained from ED for various systems $N = 16,18,20$ and $N = 32$ from Ref. [3]. For the SCBA $N \leqslant 64\times 64$, $\gamma = 0.999$ and note that delta-function contributions at $\boldsymbol{k} = \pm \boldsymbol{k}_0$ are not shown. (a) $t$–$J$ model, $t' = 0$, (b) $t$–$t'$–$J$ model with $t' = \pm t/4$ for $\boldsymbol{k} \in [(-\pi, -\pi) \to (\pi,\pi)]$, and (c) for $\boldsymbol{k} \in [(-\pi,\pi) \to (\pi, -\pi)]$.

proportional to the quasiparticle pole residue, $Z_{\boldsymbol{k}_0}$, but *not shown* in the figures. The comparison of the SCBA with the ED results shows a quantitative agreement, however, a surprising observation is that $n_{\boldsymbol{k}}$ in the SCBA exhibits a discontinuity for momenta $\boldsymbol{k} \sim \boldsymbol{k}_0, \boldsymbol{k}_0 + (\pi,\pi)$ [7]. We interpret this result as an indication of an emerging *large* Fermi surface at $\boldsymbol{k} \sim \pm \boldsymbol{k}_0$ indicating the coexistence of two apparently contradicting FS scenarios in EMDF of a single hole in an AFM. On the one hand, the $\delta$-function contributions seem to indicate that at finite doping a delta-function might develop into small FS (hole pockets). On the other hand, the discontinuities at $\boldsymbol{k} = \boldsymbol{k}_0$, $\boldsymbol{k}_0 + (\pi,\pi)$ are more consistent with infinitesimally short arcs (two points) of an emerging large FS.

In Fig. 1(b) and (c) we also present the results for the $t$–$t'$–$J$ model. (i) The effect of *negative* NNN $t' = -t/4$ is relatively weak: the GS momentum remains at $\boldsymbol{k}_0 = (\pi/2,\pi/2)$. Otherwise results are similar to the $t' = 0$ case. (ii) *Positive* NNN hopping matrix elements $t' = t/4$: the GS is now twofold degenerate, with the momenta at corners of the AFM zone, e.g., $\boldsymbol{k}_0 = (\pi,0)$. All results agree with the SCBA method.

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