Does the Two-Dimensional $t$-$J$ Model have Hole Pockets?

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We have calculated the high temperature series for the momentum distribution function $n_k$ of the 2D $t$-$J$ model to twelfth order in inverse temperature. By extrapolating the series to $T = 0.2 J$ we investigate the possibility of hole pockets in the $t$-$J$ model. We find no indication of hole pockets at an electron density of $n = 0.9$ with $J/t = 0.5$ or $J/t = 1.0$.

The locus in momentum space of low energy single particle excitations is of prime importance for what it can tell us about the nature of the low energy degrees of freedom of the two dimensional $t$-$J$ model. Two alternatives have been widely discussed: a) a large Fermi surface consistent with Luttinger’s theorem for a nearly half filled band and b) small hole pockets centered around $(\pi/2, \pi/2)$, similar to a lightly doped valence band in a semiconductor [1]. From the available experimental data which of these is correct for high temperature superconductors, if either, is still an open question. Angle resolved photoemission experiments and neutron scattering experiments generally support a large Fermi surface. However, transport measurements are more consistent with a small number of positive charge carriers, in line with b) above. The motivation for hole pockets centered around $(\pi/2, \pi/2)$ came from theoretical studies of a single hole in a Néel background [1]. More recently, hole pockets have been discussed theoretically [2,3] and experimentally [4] in regard to shadow bands.

A detailed investigation of hole pockets requires the complete single particle spectral function. However, Duffy and Moreo [3] have discussed the signature of hole pockets in $n_k$ for a spin density wave mean-field approximation to the Hubbard model [2]. Within this approach a deep notch centered on $(\pi/2, \pi/2)$ develops in $n_k$ for low enough temperatures. Below we investigate the possibility of this type of hole pocket in the 2D $t$-$J$ model.

To investigate the nature of the occupied states for the 2D $t$-$J$ model we calculated the high temperature series for the momentum distribution $n_k$ to twelfth order in inverse temperature. This is an extension of an earlier series calculation by Singh and Glenister [3] to eighth order in inverse temperature. Our series coefficients agree with theirs through eighth order. The Hamiltonian for the $t$-$J$ model is given by

$$H = -t \sum_{\langle ij \rangle, \sigma} \left( c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} \right) + J \sum_{\langle ij \rangle} S_i \cdot S_j,$$

with the constraint of no double occupancy. The definition of the single spin momentum distribution function is

$$n_k = \sum_r n_r e^{i \mathbf{k} \cdot \mathbf{r}},$$

with $n_r = \langle c_{\mathbf{r} \sigma}^\dagger c_{\mathbf{r} \sigma} \rangle$. The series coefficients are generated in coordinate space with the Fourier transform to momentum space done exactly. The resulting series coefficients in momentum space are exact functions of the wave vector. By extrapolating the series to low temperatures and using the exact momentum dependence of the series we can probe the momentum dependence of $n_k$ with high precision.

To reach low temperatures we need to analytically continue the series for $n_k$. A standard way to do this is to use Padé approximants. For $n_k$ the straightforward application of Padés does not work very well. One way to improve the convergence of Padé approximants is to change the expansion variable to move the poles of the Padés farther from the origin [5]. Exactly what change of variable to choose is difficult to know for unknown functions. However, if the Padés converge well for a certain choice of parameters for $n_k$, we can calculate the ratio of $n_k$ for this choice of parameters to $n_k$ for another choice of parameters, generally close by. This gives a much simpler function to extrapolate with the Padés and much better convergence. Once the extrapolation is done the desired result can be obtained by multiplying the ratio by the known function. For $n_k$ it’s easiest to fix $n$, $J$ and $t$ and vary $\mathbf{k}$. This is the method of extrapolation used to obtain the data below.

Hole pockets are expected to be most prominent for the underdoped cuprates [1], $\delta \lesssim 15\%$. To check this we fix the electron density as $n = 0.9$ ($\delta = 10\%$). The coupling constant ratio is less well known, but is typically chosen to be around $J/t \sim 0.4$. As a representative value we use $J/t = 0.5$. Since strong antiferromagnetic correlations are expected to promote hole pocket formation we have also investigated $n_k$ for $J/t = 1.0$. The results of our calculations are shown in Fig. 1. The momentum distributions for the two values of $J/t$ are quite similar, with $n_k$ slightly larger near $(\pi, \pi)$ for $J/t = 1.0$. Since for both values of $J/t$ $n_k$ must satisfy the sum rule $\sum_k n_k = n/2$ there must be a corresponding redistribution of weight for $n_k$ at $J/t = 1.0$ elsewhere in the Brillouin zone. To
check this would require a more complete set of data than presented here. The main feature of both curves presented in Fig. 1 is that \( n_k \) for the parameters chosen here is a smooth function of \( k \). Our results also satisfy the inequality \( n_k \leq (1 + \delta)/2 \), with \( n_k = 0.55 \) for \( k = 0 \) and \( n_k \) monotonically falling with increasing \( k \).

From the smooth, monotonic \( k \) dependence of \( n_k \) there is clearly no indication of hole pockets near \((\pi/2, \pi/2)\). There is also no obvious sign at \( T = 0.2J \) of a quasiparticle discontinuity. Where to look for a quasiparticle discontinuity is a subtle problem when \( T \neq 0 \). From Fig. 1 we can see that \( n_k = 1/2 \) is at a different wave vector than where \( n_k \) has its maximum gradient, so we do not obtain a unique \( k_F \). This problem will be addressed in a future publication.

![Graph](image.png)

**FIG. 1.** The momentum distribution \( n_k \) plotted versus wave vector \( k = (\pi x, \pi y) \) along the diagonal of the square Brillouin zone. The electron density is fixed at \( n = 0.9 \) and the extrapolated temperature is \( T/J = 0.2 \) (room temperature). a) \( J/t = 0.5 \) b) \( J/t = 1.0 \).

The momentum distribution for strongly correlated 2D electrons has been studied previously by a range of numerical methods. Stephan and Horsch [6] studied the 2D \( t-J \) model using the Lanczos algorithm at \( T = 0 \) on 16 × 20 site clusters. They had relatively few \( k \)-points available due to the small cluster sizes, but their results are clearly consistent with a large Fermi surface. The previous high temperature series work [5] presented results for a range of dopings at \( T = 1.0J \), all of which are consistent with a large Fermi surface. Quantum Monte Carlo has been used to study \( n_k \) in the Hubbard model [9]. Results for \( n = 0.87, U/t = 4, \) and \( \beta t = 6 \) on a \( 16 \times 16 \) lattice are also consistent with a large Fermi surface.

Recently, the question of hole pockets in the Hubbard model has been reexamined [3], with the suggestion that hole pockets would not show up until fairly low temperatures of order \( \beta t \sim 10 \) for \( U/t \sim 8 \). While the \( t-J \) model and the Hubbard model are only directly comparable for \( J/t \ll 1 \), our data at \( J/t = 0.5 \) can be approximately compared to the Hubbard data using the relation \( J/t = 4t/U \). For \( J/t = 0.5 \) we expect results similar to those for the Hubbard model at \( U/t = 8 \). The temperature of our results at \( J/t = 0.5 \) is \( T = 0.2J = 0.1t \). This is low enough that we would expect to see an effect due to hole pockets of the type discussed for the Hubbard model [3]. Our current results do not show any indication of hole pockets of this type.

In summary, we calculated a twelfth order high temperature series for the momentum distribution \( n_k \) of the 2D \( t-J \) model. By extrapolating the series to \( T = 0.2J \) we examined \( n_k \) near \( k = (\pi/2, \pi/2) \), looking for hole pockets centered at this wave vector. We find a smooth monotonic wave vector dependence for \( n_k \) through \((\pi/2, \pi/2)\), with no indication of hole pockets.

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