Non-Fermi-Liquid-Like Behavior in The Two-Dimensional $t - J$ Model

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The spin, charge and pairing correlation functions for the ground state of two-dimensional $t - J$ model are calculated by using the power method which projects out the ground state from a variational wave function. “Exact” results are obtained for $10 \times 10$ and $8 \times 8$ lattices with low particle densities. The results are surprisingly similar to that of one-dimensional $t - J$ model. The phenomenology is almost perfectly correlated with the concept of Tomonaga-Luttinger liquid and it is incompatible with traditional Fermi liquid theory.

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It has been well accepted now that the normal state of the high temperature superconductors is not an ordinary Fermi liquid (FL) [1]. For the last several years Anderson [2,3] has been promoting the idea of a Tomonaga-Luttinger liquid (TLL) [4]. TLL is shown by exact theories [5] and numerical studies [6,7] to be the ground state of the Hubbard model and $t-J$ model in one dimension. But until now there is no evidence that the $t-J$ model or any other model in two dimensions will indeed have such a ground state.

In this letter we present numerical results for the ground-state correlation functions calculated by the power method [7] in the low particle-density region. The calculations are done on an $8 \times 8$ square lattice and on a $10 \times 10$ lattice. The overall data have a surprisingly similarity with what we have found in one-dimension [7]. The variations of the spin, charge and pairing correlation functions with the coupling constant $J/t$ can be easily understood by borrowing the concept of the correlation exponent $K_\rho$ in one dimension. TLL provides a consistent interpretation of all the observed features in these correlation functions [3].

Exact results in the ground state of the $t-J$ Hamiltonian have been obtained by diagonalizing small lattices such as 16 or 18 sites [8,9]. Various variational approaches have been used to study larger lattices [10-11]. Recently, Valenti and Gros [12] generalized a trial wave function used by Hellberg and Mele [13] in one dimension to study the two-dimensional $t-J$ model. This wave function (HMVG) is shown to be a TLL in two dimensions. Due to the nature of the variational approach it is difficult to assess how close the variational state is to the true ground state.

Here we adopt a ground-state projection method that systematically improves the variational wave function and provides quantitative information about the ground state. This method which we shall refer to as the power method is a simplified version of the Green’s function Monte Carlo method.
The mathematical idea is quite simple. Given a wave function $|\psi\rangle$ that is not orthogonal to the ground state of a Hamiltonian $H$, applying the operator $(W - H)^p$ to $|\psi\rangle$ will project out the ground state as the power $p$ approaches infinity. The constant $W$ is chosen such that all the excited state with energy $E_i$ satisfies the relation $|W - E_i| < |W - E_g|$, where $E_g$ is the ground state energy. For the $t-J$ Hamiltonian, it is sufficient to choose $W = 0$. The numerical technique we use to implement the power method is a combination of the variational Monte Carlo (VMC) method and the Neumann-Ulam matrix method [16]. Specific details of our method can be found in reference 7.

All the data presented in this paper is obtained by averaging ten to twenty independent groups. Each group usually consists of one to two thousands starting configurations determined by the chosen trial wave function. Each starting configuration then would produce a couple hundred paths. The calculations are all done in workstations with average running time about a day or less. Obviously, the amount of computer time required is very sensitive to the size of the system, the choice of the initial trial wave function and how many powers required. In two dimensions this method usually cannot be carried out for very large powers because of the Fermion “sign” problem [17]. Fortunately, for low particle density the sign problem is not severe. For power equals to twenty, the negative terms are only about six percent of the total.

This method has been successfully applied to study the $t-J$ model in one dimension [7,18]. The calculated results of the static structure factors of longitudinal spin, $S(k)$; of charge, $D(k)$; and of pairing, $P(k)$, have a power-law decay in real-space as predicted by the TLL [5,6]. All correlation functions are determined by a dimensionless correlation exponent $K_\rho$:

$$
\langle S_z(r)S_z(0) \rangle \sim A_0 r^{-2} + A_1 \cos(2k_F r)r^{-(1+K_\rho)}, \quad (1)
$$

$$
\langle n(r)n(0) \rangle \sim B_0 r^{-2} + B_1 \cos(2k_F r)r^{-(1+K_\rho)} + B_2 \cos(4k_F r)r^{-4K_\rho}, \quad (2)
$$
where \( r \gg 1 \) and the singlet pairing operator \( \Delta(r) = C_{r\uparrow}C_{r+1\downarrow} - C_{r\downarrow}C_{r+1\uparrow} \). For \( J/t < 2 \), \( K_\rho \) is less than 1. This is the repulsive TLL where spin-density-wave (SDW) correlation dominates as reflected by a cusp in \( S(k) \) at \( k = 2k_F \). In this region pairing correlation is suppressed and charge structure factor has a maximum at zone boundary \( k = \pi \). For \( J = 2 \), \( K_\rho \) is very close to 1 and we have the Fermi liquid behavior for all the correlation functions \[19\]. When \( J \) is increased above the value of 2, pairing correlation becomes dominant with \( K_\rho > 1 \). This is the attractive TLL. \( P(k) \) has an upward cusp at \( k = 0 \) and a dip at \( k = 2k_F \). The larger the \( J \) value the stronger are these effects.

In order to make sure the final result is independent of the choice of starting trial wave functions we usually use more than one wave function. In two dimensions we use the Gutzwiller wave functions, GWF \[20\], and HMVG \[12\]. GWF is just an ideal Fermi gas state satisfying the constraint of no double occupancy at any site. The function HMVG is essentially of the same form as GWF with a Slater determinant for up-spin electrons and one for down-spin electrons. In addition to these two determinants it has a long range correlation part between all the particles: \( \Pi_{i<j} |r_i - r_j|^{\nu} \), for nearest-neighbor particles we chose \( \nu = 0 \). Clearly when \( \nu \) is positive HMVG gives more weight for particles separated far apart, hence it represents an effective repulsive interaction. On the other hand when \( \nu \) is negative an effective attractive interaction has been put into the wave function. In one dimension a similar wave function is shown by Hellberg and Mele \[7,13\] to nicely describe the repulsive and attractive TLL.

In figure 1(a) energy as a function of power is plotted for 18 particles in a 10 × 10 lattice for \( J = 0.1 \). Energy is in unit of the hopping matrix element \( t \). The empty circles are the results started with the GWF, while the filled circles started with HMVG-\( \nu = 0.03 \). Lines are guide for the eyes. The inset shows the energy of 10 particles in 64 sites as a function of power \( p \). The empty
circles are results using GWF and filled circles for HMVG-$\nu = 0.05$. Clearly the same ground state energy is obtained by applying powers of $H$ to either GWF or HMVG. The empty squares in the inset of Fig. 1(a) are results for $J = 2$ started with GWF. GWF is again very close to the true ground state for $J = 2$ just as in one dimension [19]. For $J < 2$, HMVG with positive $\nu$ gives better variational energy, hence it converges faster to the ground state. For $J > 2$, variational energy of HMVG with negative $\nu$ is also about one percent from the “true” ground state energy. The agreement is not as good for higher particle densities.

Not only the energy converged when power reaches 16, both spin and charge structure factors have also converged as shown along several directions in the Brillouin zone in Fig. 1(b) and 1(c). Starting with very different variational results of GWF shown by the dotted curves and that of HMVG shown by the solid curves, the result of applying 16 powers of $H$ are shown by the empty and filled circles using the same parameters as in Fig. 1(a). The peak at $2k_F = (0.6\pi, 0)$ in $S(k)$ is more pronounced than the results of HMVG-$\nu = 0.03$. Interestingly enough, a plateau-like structure developed in $D(k)$ for $k \geq 4k_F$. Here $4k_F$ is calculated by treating all the holes, 82 of them in this case, as spinless fermions. Both these features are observed in one dimension.

As discussed above, as far as we can tell, GWF is practically the ground state for $J = 2$ with particle densities $\frac{18}{100}$ and $\frac{10}{64}$. For $J < 2$ the ground state behaves like a repulsive TLL with a very pronounced $2k_F$ SDW correlation. $S(k)$ has peaks at $2k_F$ and $D(k)$ has its maximum at zone boundary. This is again demonstrated in Fig. 2 by the triangles which are the converged results for $J = 0.1$. Here the particle density equals $\frac{10}{64}$. In this case there are two distinct $2k_F$ vectors at $\frac{7}{4}(1, 2)$ and $\frac{7}{4}(0, 3)$ [22]. The former has been chosen to be examined in detail in Fig. 2. Circles are results of GWF which are also the converged results for $J = 2$. For $J = 3$, the converged results are denoted by
squares in Fig. 2. Just as in one dimension, $J > 2$ is the region of attractive TLL. Here SDW correlation is suppressed, $S(k = 2k_F)$ is decreased, and $D(k)$ has a peak at $2k_F$.

To illuminate this cross-over behavior from repulsive to attractive TLL as $J$ is increased above 2, we show the singlet s-wave pairing structure factor $P(k)$ in Fig. 3. The result of GWF shown by the solid line is for $J = 2$. Applying eighth power of $H$ to GWF for $J = 0.1$ and $J = 3$, we obtained the results shown by the empty and filled circles respectively. $P(k = 0)$ is strongly suppressed for $J = 0.1$, but enhanced for $J = 3$. Empty squares are the result of $J = 4$ by applying twelfth power of $H$ to a projected s-wave BCS trial wave function. The shape of the curve certainly is consistent with the that of one-dimensional TLL. According to equation (3) $P(k) \sim |k|^{\frac{1}{K_0}}$ for small $k$. Comparing results of $J = 3$ (filled squares) and $J = 4$ (empty squares) in figure 3, we can easily see that the cusp at $k = 0$ increases with the value of $J$, hence $K_0$ also increases with the value of $J$. The shape of $J = 4$ is unlike BCS-type state which has a delta function like $P(k)$. Another unique signature of TLL is that $P(k)$ has a dip at $2k_F$. Detailed examination of this behavior is shown in the inset in Fig. 3. Empty circles for $J = 0.1$ clearly do not show an increase near $k = (\pi, \pi)$ as contrast to $J = 3$ (filled circles) and $J = 4$ (empty squares).

In summary, we have presented energies and structure factors of the ground states of two-dimensional $t - J$ model calculated by the power method for 18 particles in a $10 \times 10$ lattice and 10 particles in an $8 \times 8$ lattice. As far as we know, this is the first time that such accurate numerical results have been obtained for such a larger system with strongly correlated fermions. The three structure factors, spin, charge and pairing, show very similar behavior as in one dimension. Within numerical accuracy GWF seems to be the ground state for $J = 2$. For $J < 2$ the ground state is very consistent with the picture of a repulsive TLL while an attractive TLL is for $J > 2$. 
The numerical results provided above cannot completely rule out other possible ground states besides TLL. But the surprising fact is that TLL provides the most natural and consistent framework to explain all the numerical results which include many special features. A simple random-phase-approximation [23] can explain a number of results but it fails to explain the pairing structure factor. This will be discussed in detail in a future publication. We have also examined the momentum distribution function, it is again consistent with TLL. But because there are only several \( k \) vectors in a particular direction it is quite difficult to make definite statements about the exponent. It will also be discussed in the future.

The similarity between our results in one and two dimensions may due to a simple reason. For low particle densities as we have studied here the Fermi surface is almost a perfect circle. Hence the Fermi velocity is in the radial direction. We suspect this may be the reason to cause the scattering along the radial direction to dominate and the system behaves like in one dimension or more precisely in half a dimension. A similar idea has been considered by Anderson [3]. The HMVG wave function which has energy within one percent of the exact ground state is certainly consistent with an isotropic TLL. When the particle density is increased, existence of other anisotropic TLL becomes an intriguing possibility. There are evidences that d-wave pairing becomes more important than s-wave [24].

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Figure Captions:

Fig. 1 (a) Energy as a function of power, (b) spin structure factor $S(\mathbf{k})$ and (c) charge structure factor $D(\mathbf{k})$ in the $k$ space along $\Gamma$-X-M-$\Gamma$ directions for 18 particles in a $10 \times 10$ square lattice for $J = 0.1$. Empty circles are results obtained starting from GWF and filled circles are from HMVG with $\nu = 0.03$. In (b) and (c) dashed and solid lines are VMC results for GWF and HMVG. The inset shows the energy as a function of power for 10 particles in an $8 \times 8$ lattice for $J = 0.1$. Empty circles are from GWF and filled circles are from HMVG-$\nu = 0.05$. Empty squares are results for $J = 2$.

Fig. 2 (a) The spin structure factor $S(\mathbf{k})$ along $\frac{\pi}{4}(1,k_y)$ direction, and (b) along $\frac{\pi}{4}(k_x,2)$ direction for an $8 \times 8$ lattice with 10 particles. (c) and (d) are corresponding charge structure factors $D(\mathbf{k})$. Triangles are for $J = 0.1$, circles are for $J = 2$ and squares for $J = 3$. $k_x$ and $k_y$ are in unit of $\frac{\pi}{4}$.

Fig. 3 The pairing correlation $P(\mathbf{k})$ along $(1,1)$ direction for 10 particles in an $8 \times 8$ lattice. Solid line is the result of GWF. Empty and filled circles are for $J = 0.1$ and for $J = 3$, respectively, starting from GWF with power= 8. Empty squares are for $J = 4$ and power= 12 starting from a projected s-wave BCS state. The detail for $k > 2k_F$ is shown in the inset. Along $(1,1)$ direction, $(\pi, \pi)$ is closest to $2k_F$. 