Violation of Luttinger’s Theorem in the Two-Dimensional $t$-$J$ Model

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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 $T = 0.2J$ we searched for a Fermi surface of the 2D $t$-$J$ model. We find that three criteria used for estimating the location of a Fermi surface violate Luttinger’s Theorem, implying the $t$-$J$ model does not have an adiabatic connection to a non-interacting model.

Models for two-dimensional strongly correlated electrons play a central role in attempts to understand high temperature superconductors. However, the 2D models themselves are at present poorly understood. One of the main points of interest in studies of 2D strongly correlated electrons is how similar the 2D models are to Fermi liquid theory, the standard model for conventional metals. Many-body calculations for conventional metals are generally perturbative, assuming an adiabatic relation to a non-interacting model, with low energy excitations describable by quasiparticles.

By summing a perturbative expansion to all orders Luttinger was able to show that a sharp Fermi surface can exist for interacting electrons. He defined the Fermi surface to be the locus of points in $k$-space where the renormalized single particle energy is equal to the zero temperature chemical potential $E_{F} = \mu$. This requires the imaginary part of the retarded self-energy to vanish on the Fermi surface. Luttinger was able to show that $\text{Im}\Sigma_{\text{ret}}(\omega) \propto (\omega - \mu)^{2}$, satisfying this requirement. An immediate consequence of this perturbative calculation is that the volumes (areas in 2D) enclosed by the interacting and non-interacting Fermi surfaces are the same, a statement generally known as Luttinger’s Theorem.

Using high temperature series we investigated the momentum distribution function for the 2D $t$-$J$ model on a square lattice, with the Hamiltonian for the $t$-$J$ model given by

$$ H = -tP \sum_{\langle ij \rangle, \sigma} \left( c_{i\sigma}^{\dagger} c_{j\sigma} + c_{j\sigma}^{\dagger} c_{i\sigma} \right) + J \sum_{\langle ij \rangle} \mathbf{S}_{i} \cdot \mathbf{S}_{j}, \quad (1) $$

where the sums are over pairs of nearest neighbor sites and the projection operators $P$ eliminate from the Hilbert space states with doubly occupied sites. We calculated the high temperature series for the momentum distribution function to twelfth order in inverse temperature $\beta = 1/k_{B}T$, extending a previous eighth order calculation by Singh and Glenister. The definition of the single spin momentum distribution function is

$$ n_{k} = \sum_{r} n_{r} e^{i k \cdot r}, \quad (2) $$

with $n_{r} = \langle c_{0\sigma}^{\dagger} c_{r\sigma} \rangle$. For the calculations reported here we fix $J/t = 0.4$ and the electron density $n = 0.8$. A wider range of parameters will be explored in a future publication.

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. However, 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 functional form before calculating Padés. Exactly which change to make is difficult to know for unknown functions. One way to proceed is to use the function itself as a scaling function. To do this we first form the high temperature series for the ratio of two values of $n_{k}$ with the two $k$-points closely spaced and all other parameters the same. This is an exact calculation using the exact coefficients we have for $n_{k}$. The series for the ratio is then analytically continued using Padé approximants down to $T = 0.2J$ (for $J = 1500$ K this is $300$ K). At each temperature all of the ratios are referenced back to the zone center with an absolute scale for $n_{k}$ set by enforcing the sum rule $\sum_{k} n_{k} = n/2$. Using this technique we collected data for $n_{k}$ at 1326 $k$-points in the irreducible wedge of the square Brillouin zone for five temperatures $T/J = 0.2, 0.4, 0.6, 0.8$ and 1.0. The $k$-points have a uniform spacing of $\pi/50$ for $k_{x}$ and $k_{y}$. The accuracy of the $n_{k}$ calculation varies with $k$, but for $T = 0.2J$ is approximately $5\%$, for $T = 0.4J$ approximately $3\%$ and for higher temperatures $1\%$ or less.

In analyzing our results our main goals were to search for a possible Fermi surface of the 2D $t$-$J$ model and compare its area to the area of the tight-binding model Fermi surface to check Luttinger’s Theorem. Since we cannot reach $T = 0$, where the Fermi surface is defined by a sharp discontinuity in $n_{k}$, we consider three criteria which can be calculated for non-zero temperature and might be expected to smoothly approach the $T = 0$ Fermi surface as $T \rightarrow 0$. The curves in $k$-space we investigated are defined by i) $n_{k} = 1/2$, ii) $dn_{k}/dT = 0$ and iii) $|\nabla_{k} n_{k}|$ maximal.

A comparison of the locus in $k$-space where $n_{k} = 1/2$...
for the $t$-$J$ model at $T = 0.2J$ to the tight-binding model Fermi surface is shown in Fig. 1. The area enclosed by the $t$-$J$ model curve is smaller than the area of the tight-binding model Fermi surface. This difference is not due to non-zero temperature. Fig. 2 shows the temperature dependence of the $t$-$J$ model $n_k$ for $k_F = (0.4266\pi, 0.4266\pi)$, the Fermi momentum of the tight-binding model on the zone diagonal. Clearly $n_k$ for the $t$-$J$ model with this momentum remains below $1/2$ for all temperatures. The insert in Fig. 2 shows the temperature dependence of the chemical potential $\mu(T)$ for the $t$-$J$ model with the same parameters as for $n_k$. The chemical potential shows little variation for $T \approx J$, appropriate for a degenerate Fermi system, with $\mu \approx 1.66t = 4.15J$.

![Fig. 1. Comparison of the tight-binding Fermi surface (dashed line) to the locus of $k$-points for the 2D $t$-$J$ model where $n_k = 1/2$ at $T = 0.2J$ (solid line), both at an electron density of $n = 0.8$. The area enclosed by $n_k = 1/2$ for the $t$-$J$ model does not satisfy Luttinger’s Theorem.](image)

This comparison alone is not sufficient to claim a violation of Luttinger’s Theorem. In the absence of particle-hole symmetry $n_k$ need not equal 1/2 on the Fermi surface [7]. The $n_k = 1/2$ criterion for the Fermi surface has been widely applied in the past [3] and is the simplest criterion to check before doing more detailed calculations. Our $k$-resolution allows us to distinguish $n_k = 1/2$ for the $t$-$J$ model from the Fermi surface of the tight-binding model with approximately three data points separating the two curves. Previous calculations on small clusters [2] did not have sufficient $k$-resolution to make this distinction.

An improved criterion for locating a Fermi surface has been proposed by Randeria et al. [2]. They proposed that the Fermi surface be identified with the locus of $k$-points where the temperature derivative of $n_k$ is stationary: $dn_k/dT = 0$. While the high temperature series for $dn_k/dT$ can be calculated directly from the series for $n_k$, the resulting series is too short to be extrapolated to low temperatures. Alternatively, we consider the finite difference approximation $\Delta n_k/\Delta T$ where $\Delta T = 0.2J$ and $\Delta n_k$ is found by directly subtracting the two $n_k$'s for each $k$-point. Fig. 3 shows that this works very well for the tight-binding model at $T = 0.3J$. From our data we find $\Delta n_k/\Delta T$ centered on the average temperatures $T/J = 0.3, 0.5, 0.7$ and 0.9. The results are shown in Fig. 4.

![Fig. 2. Temperature dependence of the $t$-$J$ model momentum distribution function $n_k$ at the tight-binding Fermi wave vector $k_F = (0.4266\pi, 0.4266\pi)$ showing that on the tight-binding model Fermi surface the $t$-$J$ model $n_k < 1/2$ for all temperatures. Insert: Temperature dependence of the $t$-$J$ model chemical potential. For $T \approx 0.3J$ the error bars are the width of the line.](image)

The results shown in Fig. 4 have three surprising features i) the area enclosed by the curve where $\Delta n_k/\Delta T = 0$ is larger than the area enclosed by the tight-binding Fermi surface, ii) $k$-states with decreased occupancy as the temperature increases occur across a broad region in the center of the Brillouin zone and iii) at low temperatures the distribution of $k$-states with increased occupancy as the temperature increases are strongly peaked on the zone diagonal. Features ii) and iii) indicate the location of the low energy excitations in the Brillouin zone. Unlike the tight-binding model, where the low energy excitations are confined to a narrow range of $k$-points centered on the Fermi surface, the low energy excitations for the $t$-$J$ model are spread throughout the Brillouin zone. The extremal values of $\Delta n_k/\Delta T$ for the $t$-$J$ model are $\sim 10$ times smaller than for the tight-binding model, implying a relatively small density of states at any fixed momentum for the $t$-$J$ model. For $dn_k/dT = 0$ the correct Fermi surface particle-hole symmetry is required for low energies [7]. This may not be valid for the 2D $t$-$J$ model. Thus the locus of $k$-points where $dn_k/dT = 0$ may not give the true Fermi surface.

The final criterion we considered for locating a Fermi surface for the 2D $t$-$J$ model is to follow the locus of $k$-points where $|\nabla_k n_k|$ is maximal [3]. This criterion only depends on $n_k$ having a sharp discontinuity at the Fermi surface for $T = 0$. For $T > 0$ the discontinuity will be smeared out, but we still expect $|\nabla_k n_k|$ to be large near the Fermi surface since we have a degenerate Fermi system. As shown in Fig. 3 this criterion gives the proper Fermi surface for the tight-binding model. For the $t$-$J$ model we calculate $|\nabla_k n_k|$ numerically from $n_k$, with the results shown in Fig. 5.
At the lowest temperature shown in Fig. 5, $T = 0.2J$, our results have two main features i) the area enclosed by following a continuous locus of $k$-points along a ridge where $|\nabla_k n_k|$ is maximal (as indicated by the dotted line in Fig. 5) is larger than the area enclosed by the tight-binding model Fermi surface and ii) $|\nabla_k n_k|$ is strongly peaked on the zone diagonal. However, compared to the tight-binding model, the maximum value of $|\nabla_k n_k|$ for the $t$-$J$ model at $T = 0.2J$ is $\sim 10$ times smaller. The shape of the area enclosed by the dotted line in Fig. 5 is similar to that for the tight-binding model with a next-nearest neighbor hopping term, but this modification to the tight-binding Hamiltonian can only change the shape of the Fermi surface, not its area. Thus our results for the $t$-$J$ model cannot be modeled as a band of non-interacting electrons with a modified band structure.

The main result of our calculation is that the 2D $t$-$J$ model violates Luttinger’s Theorem. This means the ground state of the 2D $t$-$J$ model is not adiabatically related to a non-interacting model. Also, the distribution of low energy excitations revealed by $\Delta n_k/\Delta T$ suggests that quasiparticles cannot describe all of the low energy degrees of freedom of the 2D $t$-$J$ model. However, our results are not sufficient to uniquely determine the ground state of the 2D $t$-$J$ model.

The simplest way to not have an adiabatic connection to non-interacting electrons is for the 2D $t$-$J$ model to have an ordered ground state with a different symmetry than non-interacting electrons. The low temperature growth of peaks in $\Delta n_k/\Delta T$ and $|\nabla_k n_k|$ suggests some kind of order is developing in the $t$-$J$ model. The entropy of the $t$-$J$ model also starts to decrease at $T \sim J$. At present it is not possible to determine the precise nature of this order. We know from the spin correlation function and the antiferromagnetic correlation length that...
we do not have long range spin order. Concomitantly, we do not observe hole pockets in $n_{k}$ [13]. For the $t$-$J$ model the charge fluctuations are suppressed, with no indication of short wavelength structure in the charge density [14]. The location of peaks in $\Delta n_{k}/\Delta T$ and $|\nabla_{k}n_{k}|$ along the zone diagonal is consistent with the location of gap nodes for $d_{x^2-y^2}$ superconducting fluctuations. If this is correct, superconducting fluctuations at low temperatures are developing in the 2D $t$-$J$ model from a higher temperature state which cannot be described as a Fermi liquid. For $T \sim J$ the $t$-$J$ $n_{k}$ can be modeled by assuming spin-charge separation [14,15]. However, there is no clear reason for peaks to appear in $\Delta n_{k}/\Delta T$ or $|\nabla_{k}n_{k}|$ for a spin-charge separated state.

Other theoretical approaches have found results similar to our data. In particular SU(2) gauge theory calculations [10] and phenomenological models of preformed pairs [17] or of a d-wave ground state [13] find Fermi arcs centered on the zone diagonal and the Fermi surface gapped or destroyed by strong scattering near $k = (\pi, 0)$. These theories are motivated by the pseudogap observed in ARPES [19]. The largest value of $|\nabla_{k}n_{k}|$ and the sharpest region for $\Delta n_{k}/\Delta T = 0$ form arcs centered on the zone diagonal with the same outward curvature as the ARPES data. However, the maximum value of $|\nabla_{k}n_{k}|$ is substantially smaller than what might be expected for a true discontinuity unless there is an energy scale in the $t$-$J$ model smaller than 0.2$J = 300K$. Our data also are similar to the “cold spots” proposed by Ioffe and Millis [20] and quasiparticle decay as discussed by Laughlin [21], plus calculations for $t$-$J$ ladders that show gapped and non-gapped features in $n_{k}$ [22].

ARPES experiments do not directly measure $n_{k}$, though attempts have been made to integrate the ARPES data over frequency, giving a value proportional to $n_{k}$, but with an unknown scale factor [1]. We can make a qualitative comparison of our results to features of the ARPES data [22] i) $|\nabla_{k}n_{k}|$ maximal gives a locus in $k$-space with the same shape as the Fermi surface found in ARPES experiments, ii) without Luttinger’s Theorem, the peaks observed by ARPES in the normal state [4] do not have to be quasiparticles and iii) we see a large region with low energy excitations, similar to the flat background extending up to the chemical potential in ARPES data [13, 19, 23].

In conclusion, we find that the $t$-$J$ model violates Luttinger’s Theorem. Using $|\nabla_{k}n_{k}|$ as the least biased way to search for a Fermi surface we find the area enclosed by the curve where $|\nabla_{k}n_{k}|$ is maximal to be larger than the area enclosed by the Fermi surface of the tight-binding model. We also found structure in the low energy excitations of the 2D $t$-$J$ model which might be due to $d_{x^2-y^2}$ superconducting fluctuations.

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[1] T. M. Rice in Proceedings of the Les Houches Summer School, Session LXVI, ed. by B. Duçot and Z. Zinn-Justin (Elsevier, Amsterdam, 1995), p. 19.
[2] D. Pines and P. Nozières, The Theory of Quantum Liquids, vol. 1 (Addison-Wesley, Redwood City, CA, 1989).
[3] J. M. Luttinger and J. C. Ward, Phys. Rev. 118, 1417 (1960); J. M. Luttinger, Phys. Rev. 119, 1153 (1960).
[4] J. M. Luttinger, Phys. Rev. 121, 942 (1960).
[5] R. R. Singh and R. L. Glenister, Phys. Rev. B46, 14313 (1992).
[6] A. J. Guttmann in Phase Transitions and Critical Phenomena, vol. 13, ed. by C. Domb and J. L. Lebowitz (Academic, San Diego, 1989). p. 1.
[7] M. Randeria et al., Phys. Rev. Lett. 74, 4951 (1995); M. Randeria and J.-C. Campuzano, cond-mat/9709101.
[8] J.-C. Campuzano et al., Phys. Rev. B53, R14737 (1996).
[9] W. Stephan and P. Horsch, Phys. Rev. Lett. 66, 2258 (1991); E. Dagotto, E. F. Ortolani and D. Scalapino, Phys. Rev. B46, 3183 (1992); A. Moreo et al., Phys. Rev. B41, 2313 (1990).
[10] W. O. Putikka in Proceedings of the 10th Anniversary HTS Workshop, ed. by B. Batlogg, et al. (World Scientific, Singapore, 1996), p. 527.
[11] R. R. Singh and R. L. Glenister, Phys. Rev. B46, 11871 (1992).
[12] W. O. Putikka, J. Phys. Chem. Solids 56, 1747 (1995).
[13] W. O. Putikka, M. U. Luchini and R. R. P. Singh, to be published.
[14] W. O. Putikka, R. L. Glenister, R. R. P. Singh and H. Tsunetsugu, Phys. Rev. Lett. 73, 170 (1994).
[15] W. O. Putikka in Physical Phenomena at High Magnetic Fields II, ed. by Z. Fisk, et al. (World Scientific, Singapore, 1996), p. 567.
[16] X. G. Wen and P. A. Lee, Phys. Rev. Lett. 80, 2193 (1998).
[17] V. B. Geshkenbein, L. B. Ioffe and A. I. Larkin, Phys. Rev. B55, 3173 (1997).
[18] J. R. Engelbrecht, et al., cond-mat/9705166.
[19] M. R. Norman, et al., cond-mat/9710163.
[20] L. B. Ioffe and A. J. Millis, cond-mat/9801092.
[21] R. B. Laughlin, cond-mat/9608062v2.
[22] T. M. Rice, et al., cond-mat/9706147.
[23] Z.-X. Shen and D. S. Dessau, Phys. Rep. 253, 2 (1995).