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Nishimoto, S.; Ohta, Y.; Eder, R

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Landau mapping and Fermi-liquid parameters of the two-dimensional *t*-*J* model

S. Nishimoto and Y. Ohta
Department of Physics, Chiba University, Inage-ku, Chiba 263, Japan

R. Eder
Department of Solid State Physics, University of Groningen, 9747 AG Groningen, The Netherlands

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An exact-diagonalization technique on small clusters is used to study the momentum distribution function $n(\mathbf{k})$ of the lightly doped t-J model in two dimensions. We find that $n(\mathbf{k})$ can be decomposed into two components with bosonic and fermionic doping dependence. The bosonic component originates from the incoherent motion of holes and has no significance for low-energy physics. For the fermionic component we explicitly perform the one-to-one Landau mapping between all low-lying states of the t-J model and those of a system of spin-1/2 quasiparticles and extract the quasiparticle dispersion and Landau parameters. [S0163-1829(98)50810-7]

Despite considerable experimental efforts, the Fermi-surface topology of cuprate superconductors continues to pose an intriguing and not really well-understood problem. While it seemed to be settled that the Fermi surface of these materials is simply the one predicted by local-density approximation (LDA) calculations, with a moderate correlation narrowing of the bandwidth, recent developments in photoelectron spectroscopy, like the discovery of the shadow bands[1] or the temperature dependent pseudogap at $(\pi,0)$,[2] have challenged this point of view. There is moreover the long-standing problem that Fermi-liquid-like calculations based on the LDA Fermi surface cannot describe the dependence of either Hall constant or dc resistivity on the hole concentration δ; both quantities consistently suggest a carrier density $\propto\delta$,[3] rather than $\propto(1-\delta)$ as it would be for the LDA Fermi surfaces. On the other hand, taking the shadow bands as a true part of the Fermi surface, which then would have the topology of elliptical hole pockets centered on $(\pi/2,\pi/2)$, would immediately lead to complete accord between Fermi-surface topology and transport properties in the framework of a very simple Fermi-liquid-like picture.[4] While such a picture is thus quite appealing, clear experimental evidence for hole pockets has not been found so far.

It is the purpose of the present paper to address the problem of Fermi-surface topology of cuprates theoretically, by studying the two-dimensional t-J model, the simplest strong correlation model which may give a realistic description of the CuO_2 plane. Thereby we search for a ''dip fine structure'' in the electron momentum distribution (EMD) function $n_\sigma(\mathbf{k})=\langle c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\rangle$ (for simplicity we will omit the spin index unless it is indispensable). The main problem which has to be overcome in extracting the fermiology from $n(\mathbf{k})$ is the presence of extended incoherent continua in the photoemission spectra of this model. Since $n(\mathbf{k})$ is the 0th moment of the photoemission spectrum, it is composed of two parts: $n(\mathbf{k})=Z\Theta(\omega_{\rm QP}-E_{\rm F})+\int d\omega A_{\rm inc}(\mathbf{k},\omega)$, where $\omega_{\rm QP}$ and Z denote the quasiparticle dispersion and weight, and $A_{\rm inc}(\mathbf{k},\omega)$ the incoherent high-energy part of the spectral function. In general the latter part has a $\mathbf{k}$ dependence of its own, which must be distinguished from the Fermi-surface discontinuities. In principle, $A_{\rm inc}(\mathbf{k},\omega)$ should be a smooth function of $\mathbf{k}$, so that a sufficiently good momentum resolution would allow us to distinguish the steplike variations at $E_{\rm F}$; this however is out of the question with the relatively coarse $\mathbf{k}$ meshes available in cluster diagonalizations. In the following we will show however that the incoherent component is practically identical for all low-energy states with fixed hole number. This allows us to subtract it off and thus make a dip fine structure in $n(\mathbf{k})$ visible. The latter originates from the $\mathbf{k}$-space distribution of the holelike *quasiparticles* rather than the bare electrons and can be used to establish the Landau mapping between the exact low-energy eigenstates of the t-J model to those of a suitably chosen quasiparticle Hamiltonian. In this way we obtain dispersion, Landau parameters, and statistics of the elementary excitations.

At half filling the EMD for the t-J model is a constant: $n(\mathbf{k})=1/2$. This is similar to a band insulator where we have $n(\mathbf{k})=1$. Then, in the band insulator, the EMD for a state with a single hole, momentum $\mathbf{k}_0$, and spin σ_0 would be $n_\sigma(\mathbf{k})=1-\delta_{\mathbf{k},-\mathbf{k}_0}\cdot\delta_{\sigma,\bar{\sigma}_0}$, i.e., a constant with a dip at $-\mathbf{k}_0$ and $\bar{\sigma}_0$. The single-hole EMD for the t-J model is however quite different as we can see in Fig. 1. To emphasize small differences, this figure shows $n_\sigma(\mathbf{k})$ with its mean value N_σ/N being subtracted (N_σ denotes the number of σ-spin electrons and N the cluster size). The dip expected at $-\mathbf{k}_0$ and $\bar{\sigma}_0$ does exist, but is quite shallow; there are also satellite dips at $-\mathbf{k}_0+(\pi,\pi)$, reflecting the strong antiferromagnetic order at half filling. More importantly, $n_\sigma(\mathbf{k})$, for both spin directions, acquires an additional, apparently smooth component, whose oscillation around the mean value is nearly independent of σ.

A surprising result can be obtained by plotting the amplitude of the smooth component, i.e., $\Delta=n(0,0)-n(\pi,\pi)$, as a function of the hole concentration δ (see Fig. 2). For δ as large as 0.2 the relation $\Delta\propto\delta$ holds with high accuracy, which is an entirely unexpected result if we adopt a free-electron-like picture, where a change of the electron density should affect $n(\mathbf{k})$ predominantly near the noninteracting Fermi surface. We could on the other hand understand this

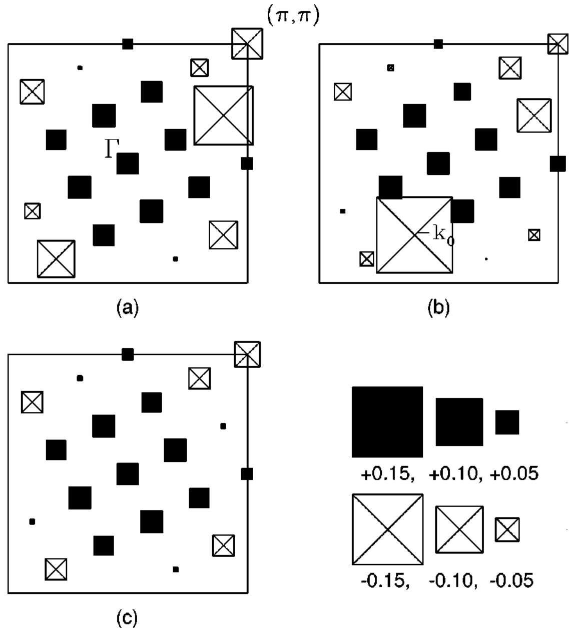

FIG. 1. EMD for the single-hole ground state of the 20-site cluster [with total momentum $\mathbf{k}_0=(\pi/5,3\pi/5)$, $S_z=1/2$, and $J/t=0.5$]. The figures show (a) $n_\uparrow(\mathbf{k})$, (b) $n_\downarrow(\mathbf{k})$, and (c) $n_{\rm inc}(\mathbf{k})$, in the entire Brillouin zone. The edge of the square centered on a given $\mathbf{k}$ point is proportional to $|n_\sigma(\mathbf{k})-N_\sigma/N|$. Positive (negative) values are indicated by black (crossed) squares, and the calibration for their magnitude is given in the bottom right figure.

result if we were to assume that each hole brings with it the same smooth contribution as the single hole in Fig. 1, so that for each hole number $n(\mathbf{k})$ contains this component times the number of holes. Such an assumption in turn is very natural[5] if we assume that the doped holes are spin bags[6] where the bare hole oscillates rapidly inside a region of reduced spin correlation. In this picture the smooth component of $n(\mathbf{k})$ comes from the (incoherent and high-energy) oscillation of the hole inside the spin bag.[5] If this high-energy motion is sufficiently decoupled from the much slower drift motion of the entire quasihole (i.e., the hole plus its dressing region), one may expect that this high-energy oscillation contributes identically to $n(\mathbf{k})$ for each quasihole, whence the scaling of

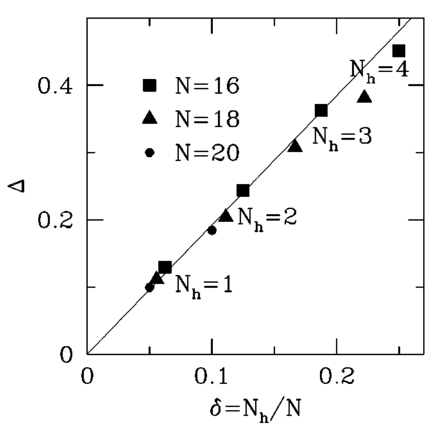

FIG. 2. Amplitude $\Delta=n(0,0)-n(\pi,\pi)$ versus hole concentration δ, for various cluster sizes N and hole numbers N_h. For odd N_h the average over spin directions has been taken. $J/t=0.4$ is used. The full line is a guide to the eye.

$n(\mathbf{k})$ with δ. In spin-charge-separation language one might say that the physical quasiparticle is a firmly bound state of spinon and holon (i.e., a holelike spin-1/2 fermion). The rapid oscillation of the bound holon then corresponds to the motion of a boson in a localized orbital, and bosons which populate a localized orbital much smaller than the cluster size trivially do have a momentum distribution proportional to the boson (=hole) density. For the same reason one may expect that the picture proposed by Lee *et al.*,[7] who modeled the charge degrees of freedom by bosons diffusing in a fluctuating magnetic field, would also give a diffuse component in $n(\mathbf{k})$ proportional to δ.

With these ideas in mind we now adopt the hypothesis that $n(\mathbf{k})$ can be decomposed into two components: (i) a smooth contribution which stems from the incoherent, bosonlike charge fluctuations on scale t, and scales accurately with δ, and (ii) a dip fine structure, where each of the holelike quasiparticles contributes to a dip which marks its position in $\mathbf{k}$ space. Thus, we write the EMD for a single-hole state as

$$n_\sigma(\mathbf{k})=\frac{N_\sigma}{N}-Z\,\delta_{\mathbf{k},-\mathbf{k}_0}\cdot\delta_{\sigma,\bar{\sigma}_0}+n_{\rm inc}(\mathbf{k}), \tag{1}$$

and try to extract an estimate for $n_{\rm inc}(\mathbf{k})$. To that end we first close the dip at $-\mathbf{k}_0$ by replacing $n(-\mathbf{k}_0)$ by that for a symmetry-equivalent $\mathbf{k}$ point; e.g., in Fig. 1 where $\mathbf{k}_0=(\pi/5,3\pi/5)$, we replace $n_\downarrow(-\pi/5,-3\pi/5)\rightarrow n_\downarrow(-3\pi/5,\pi/5)$. The satellite dips are closed in an analogous way. Subtracting now the mean value N_σ/N, we obtain the incoherent contribution $n_{\rm inc}(\mathbf{k})$, which as discussed above should correspond to the incoherent and high-energy charge oscillations of a *single* hole. For simplicity we average $n_{\rm inc}(\mathbf{k})$ over spin directions and point-group operations [see Fig. 1(c)]. Then, we expect that the EMD for an eigenstate $|\Psi_\nu\rangle$ with N_h holes (assumed to be even) takes the form

$$n(\mathbf{k})=\frac{N-N_h}{2}-Z\cdot n_{\rm coh}(\mathbf{k})+N_h\cdot n_{\rm inc}(\mathbf{k}). \tag{2}$$

Thereby the coherent part $n_{\rm coh}(\mathbf{k})$ corresponds to the EMD of N_h spin-1/2 fermions which form a state with the opposite total momentum [because $n_{\rm coh}(\mathbf{k})$ refers to *holes*], but the same spin and point-group symmetry as $|\Psi_\nu\rangle$. It can be obtained numerically by subtracting $(N-N_h)/2+N_h\cdot n_{\rm inc}(\mathbf{k})$ from the exact EMD and normalizing the remaining distribution to N_h particles.

To judge the outcome of this procedure we next have to know how the N_h quasiholes distribute themselves in $\mathbf{k}$ space for a given total momentum and spin; in other words, we need to guess the quasiparticle Hamiltonian. The generic form is

$$H=\sum_{ij\sigma} t_{ij}a_{i\sigma}^\dagger a_{j\sigma}+\sum_{ij}\,(V_{ij}n_in_j+J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j), \tag{3}$$

where $a^\dagger$ creates a quasiparticle. Below we will concentrate on the case $N_h=2$ (corresponding to $\delta\approx 10\%$ in our clusters). Then, a two-particle eigenstate of Eq. (3) with momentum $-\mathbf{k}_{\rm tot}$ and spin $S=0,1$ can always be expanded as

$$|\Psi\rangle=\sum_{\mathbf{k}}\frac{\alpha_{\mathbf{k}}}{\sqrt{2}}[a^{\dagger}_{-\mathbf{k}_{\rm tot}+\mathbf{k}\uparrow}a^{\dagger}_{-\mathbf{k}\downarrow}-(-1)^{S}a^{\dagger}_{-\mathbf{k}_{\rm tot}+\mathbf{k}\downarrow}a^{\dagger}_{-\mathbf{k}\uparrow}].$$

Solving Eq. (3) for the wave function $\alpha_{\mathbf{k}}$ gives the momentum distribution of the *quasiparticles* as $\tilde{n}(\mathbf{k})=\frac{1}{2}(\alpha_{-\mathbf{k}}+\alpha_{\mathbf{k}_{\rm tot}+\mathbf{k}})$. Depending on the sharpness of the two-particle wave function $\alpha_{\mathbf{k}}$, $\tilde{n}(\mathbf{k})$ thus may look diffuse, although there are only two quasiparticles involved. On the other hand, $\alpha_{\mathbf{k}}$ carries information not only about the dispersion of the quasiparticles, but also their interaction. Matching $\tilde{n}(\mathbf{k})$ to the dip fine structure, $n_{\rm coh}(\mathbf{k})$ obtained by the above subtraction procedure from the exact eigenstates of the t-J model should allow us to extract quite reliable information about the quasiparticle properties. We found that an excellent fit could be obtained by using a next-nearest-neighbor hopping dispersion, i.e., only the hopping integrals t_{11} and t_{20} between the second-nearest [i.e., (1,1)] and third-nearest [i.e., (2,0)] neighbors are different from zero. To avoid a proliferation of adjustable parameters we retain only nearest-neighbor density-density and exchange interactions V_{10} and J_{10},[8] but it should be kept in mind that in view of the many ways in which two ''dressed holes'' in an antiferromagnet can interact with each other,[9] this may be an oversimplified choice. The parameters obtained are then $t_{11}=0.255$, $t_{20}=0.15$, $V_{10}=-0.6375$, and $J_{10}=0.15$ (for $J/t=0.5$, in units of t). Actually, fitting the quasiparticle wave functions gives these parameters only up to an overall prefactor; the latter was obtained by a least-squares fit of the energies, but since some extremal states may have an unduly large influence in this fit, the value of the prefactor has to be viewed with some care. Our hopping parameters give a bandwidth of $W\approx 4.8J$, whereas a more likely estimate is $2J$,[8,11] and an inaccuracy of the prefactor may well be responsible for this. Independently of this, the largest interaction parameter is $V_{10}\approx W/4$, so that Eq. (3) describes a dilute system of only weakly interacting fermions.

We turn to a detailed comparison of the dip fine structure $n_{\rm coh}(\mathbf{k})$ and the quasiparticle distribution $\tilde{n}(\mathbf{k})$; see Figs. 3 and 4. Obviously the calculated coherent components $n_{\rm coh}(\mathbf{k})$ are indeed coherent, i.e., in most cases they are rather localized in $\mathbf{k}$ space and nearly zero almost everywhere in the Brillouin zone. This shows that for most $\mathbf{k}$ points our scaling hypothesis for $n(\mathbf{k})$ is correct. It should be kept in mind that for each cluster size we have subtracted one and the same estimated incoherent contribution from the exact EMD for *all* different low-energy states in the t-J model to obtain the $n_{\rm coh}(\mathbf{k})$. Next, comparing $n_{\rm coh}(\mathbf{k})$ with the EMD for the model system, a remarkable pattern matching is obvious. Among the 20 different states shown in Figs. 3 and 4 only the singlet state with $\mathbf{k}=(\pi/3,\pi/3)$ in the 18-site cluster deviates significantly. With the exception of (0,0) and (π,π), Figs. 3 and 4 comprise the lowest singlet and triplet states for all allowed momenta in both 18- and 20-site clusters. A particularly interesting case is $\mathbf{k}_{\rm tot}=(4\pi/5,2\pi/5)$ and $S=0$ in Fig. 3, where both $n_{\rm coh}(\mathbf{k})$ and $\tilde{n}(\mathbf{k})$ are sharply peaked at $\mathbf{k}_1=(3\pi/5,-\pi/5)$ and $\mathbf{k}_2=(-2\pi/5,5\pi/5)$. This state therefore must be a superposition of the two pairs $a_{\mathbf{k}_1\uparrow}a_{\mathbf{k}_1\downarrow}|{\rm vac}\rangle$ and $a_{\mathbf{k}_2\uparrow}a_{\mathbf{k}_2\downarrow}|{\rm vac}\rangle$, with nearly equal weight. Note that $2\mathbf{k}_1=(6\pi/5,-2\pi/5)$ $=(-4\pi/5,-2\pi/5)=-\mathbf{k}_{\rm tot}$, as it has to be (and similarly for $\mathbf{k}_2$). Then, in order to construct this state, the quasiparticles *must* have spin 1/2, so this is one of the states which very clearly determines the statistics of the quasiparticles [another example is the singlet $(2\pi/3,0)$ state in Fig. 4].

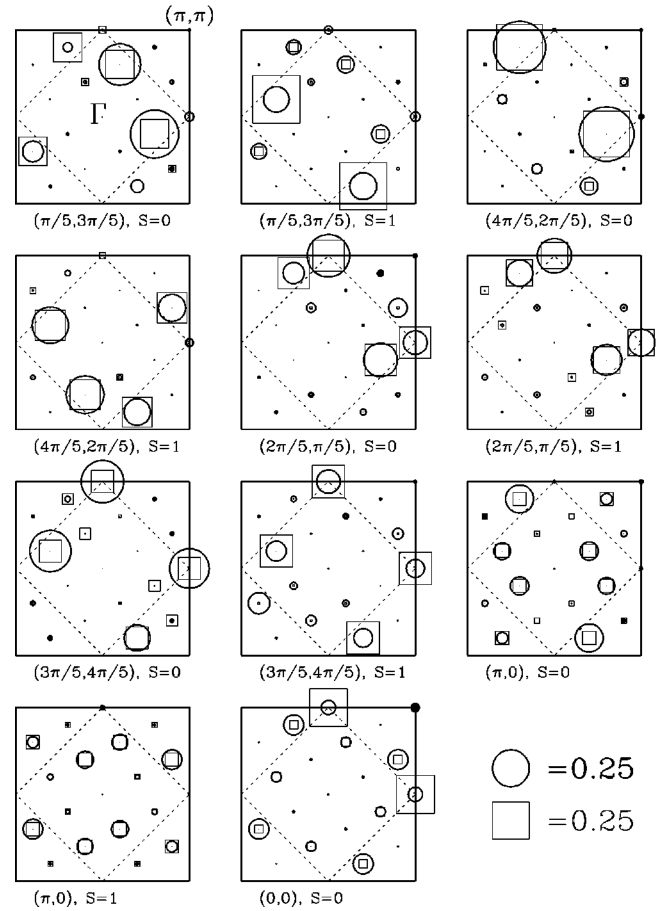

FIG. 3. Comparison between the dip fine structure $n_{\rm coh}(\mathbf{k})$ for all exact low-energy states of the 20-site cluster t-J model with two holes (circles) at $J/t=0.5$ and $\tilde{n}(\mathbf{k})=\frac{1}{2}(\alpha_{-\mathbf{k}}+\alpha_{\mathbf{k}_{\rm tot}+\mathbf{k}})$ for the Hamiltonian Eq. (3) (squares). Each graph is labeled by the total momentum and spin of the respective eigenstate and shows the entire Brillouin zone. The diameters of the circles (edges of the squares) centered on each $\mathbf{k}$ point are proportional to the respective $n(\mathbf{k})$ (see the lower right edge for the gauge). Momenta for the quasihole states are (-1) times those for the t-J model.

The problematic state with $\mathbf{k}=(\pi/3,\pi/3)$ and $S=0$ actually evolves into a charge-density wave or stripelike hole arrangement for larger values of J;[10] this may explain the discrepancies. All in all, however, the agreement is quite good, which provides clear evidence for the validity of the decomposition Eq. (2) and the quasiparticle Hamiltonian Eq. (3) with the optimized parameters.

In summary, we have investigated the EMD for all the low-energy states of the small-cluster t-J model in two dimensions. We found that each low-energy state has a state-characteristic dip fine structure superimposed over state-independent incoherent background. The dip fine structure is well fitted by the $\mathbf{k}$-space distribution of holelike spin-1/2 quasiparticles, and the incoherent background has a boson-like dependence on hole density. Using the dip structure, we have directly established the Landau mapping to a dilute

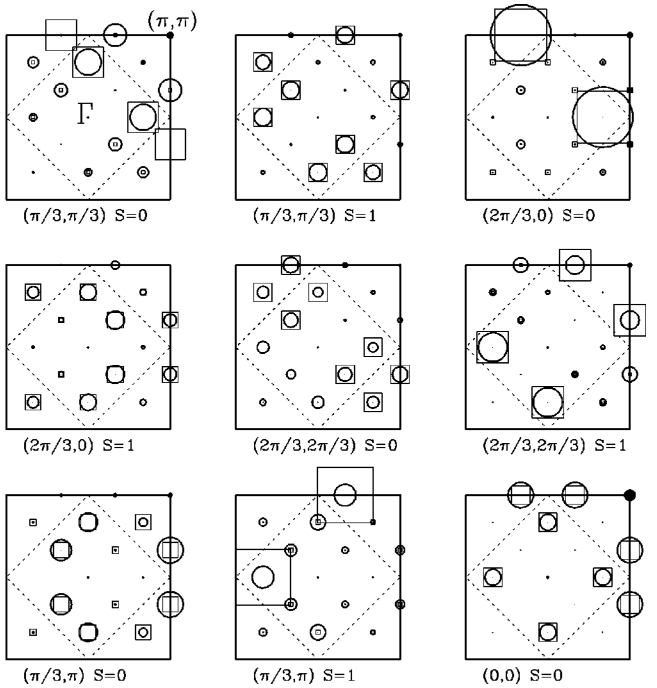

FIG. 4. Same as Fig. 3 but for two holes in the 18-site cluster.

system of weakly interacting spin-1/2 particles corresponding to the doped holes. The quasihole dispersion is dominated by next-nearest-neighbor hopping, as would be expected for dominant antiferromagnetic spin correlation,[11] but also for a ''spinon'' in a resonating-valence-bond state.[12] The interaction between quasiparticles is dominated by a nearest-neighbor attraction. Our results establish conclusively that the small clusters behave like the finite-size equivalents of a Landau Fermi liquid, in that there is a one-to-one mapping between the exact eigenstates of the interacting system and those of an interacting system of quasiparticles. The most obvious extrapolation to the infinite systems is that the same quasiparticle Hamiltonian also describes the thermodynamic limit. There is good reason to believe that the cluster diagonalization quite accurately describes short-range processes, which are the dominant ones in strongly correlated systems; for the paramagnetic regime with its very short-range spin correlations, it seems moreover plausible that longer-range processes are of little importance for either propagation or interaction of the holes, so that we believe that the extrapolation of the quasiparticle Hamiltonian from the clusters to the infinite system is a reasonable approximation. Unless the interaction between holes (which may be either the interaction intrinsic to the t-J model or the extra Coulomb repulsion) drives the system into a charge-density-wave state[10] (as may be the case in $La_{1.875}Sr_{0.125}CuO_4$), the system should thus behave like a Fermi liquid with a hole-pocket Fermi surface centered on $\mathbf{k}=(\pi/2,\pi/2)$.

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