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On the origin of the tunnelling asymmetry in the cuprate superconductors: a variational perspective

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Abstract
Through variational Monte Carlo calculations on Gutzwiller projected wavefunctions, we study the quasiparticle weight for adding and removing an electron from a high-temperature superconductor. We find that the quasiparticle weight is particle–hole symmetric at sufficiently low energy. We propose to use the tunnelling asymmetry as a tool to study the mechanism of electron incoherence in high-temperature superconductors.

1. Introduction

Scanning tunnelling microscopy (STM) plays an important role in the study of high-temperature superconductors as it provides local information on the single-particle properties with very high energy resolution. A striking feature in the STM spectra of high-temperature superconductors is the remarkable particle–hole asymmetry. The hole side of the spectrum always dominates the particle side of the spectrum in hole-doped cuprates [1].

This asymmetry is not at all surprising if we take the high-temperature superconductors as doped Mott insulators described by, for example, the t–J model. In such doped Mott insulators, an added electron has a reduced probability of contributing to the electron spectral weight in the low-energy subspace of no double occupancy. More specifically, if the hole density in the system is x, then the total spectral weight in the particle side of the spectrum is reduced to x by the no double occupancy constraint, while that in the hole side of the spectrum remains unaffected. Thus the total spectral weight is particle–hole asymmetric for small x. However, such asymmetry the total spectral weight tells us nothing about the distribution of the spectral weight in energy. To address the problem of tunnelling asymmetry in the near vicinity of the chemical potential, we need more detailed information on the low-energy excitations of the system.

Rantner and Wen addressed this issue in the slave–boson mean field theory (SBMFT) of the t–J model [2]. In their theory, the tunnelling asymmetry is attributed to the incoherent part of the electron spectrum, which is predicted to dominate the hole side of the electron spectrum and to be absent in the particle side of the electron spectrum. In the slave–boson mean-field theory, an electron is split into two parts, the fermionic spinon part that carries spin and the bosonic holon part that carries charge. The superconducting state is described by the Bose condensation of the holon in the background of Bardeen–Cooper–Schrieffer (BCS) pairing of the spinons. In the presence of the holon condensate, the electron spectrum develops a quasiparticle peak. According to the mean-field theory, the particle side of the electron spectrum is exhausted by the quasiparticle contribution, since the holon removed during the particle injection process must come from the holon condensate, while the hole side of the electron spectrum contains contributions from both the quasiparticle peak and the incoherent background, since the holon injected into the system during the particle-removing process can stay either in or out of the holon condensate. The slave–boson mean-field theory predicts that the quasiparticle weight will be reduced from the BCS mean-field value by a constant factor x and remains particle–hole symmetric. Thus the hole side of the electron spectrum is dominated by the incoherent background at small x and the majority of the tunnelling asymmetry should be attributed to the incoherent spectral weight.

Recently, Anderson and Ong addressed the same issue with a variational approach [3] but arrived at a quite different conclusion. They constructed the Gutzwiller-type variational wavefunctions for the ground state and the quasiparticle excitations of the t–J model and then treated the projection with an analytical approximation. Their theory predicted that both the particle side and the hole side of the electron spectrum are dominated by the quasiparticle contribution, which is itself particle–hole asymmetric. Thus the tunnelling asymmetry should be attributed to the coherent part rather than the incoherent part of the electron spectrum. According to their theory, for excitation energy much larger than the pairing gap, the quasiparticle weight for adding an electron into the system is a factor $\frac{2x}{1+x}$ smaller than the quasiparticle weight for removing an electron. Thus, for a system with no superconducting pairing, there will be a jump in the quasiparticle weight at the Fermi surface. At the same time, the theory predicted a non-zero quasiparticle weight for removing an electron from a half-filled system.

The problems of tunnelling asymmetry and the quasiparticle weight are also recently addressed in some other variational studies [4–7]. For example, it is proved by Yunoki that the particle side of the electron spectrum is exhausted by the quasiparticle contribution for a superconductor described by the Gutzwiller projected BCS wavefunction [5]. However, a clear understanding of the hole-like quasiparticle excitation of the Gutzwiller projected state is still absent.

In this paper, we conduct variational Monte Carlo (VMC) calculations on the Gutzwiller projected wavefunctions and find that the quasiparticle weight in the t–J model is particle–hole symmetric at sufficiently low energy, even with no superconducting pairing. Especially, we find the quasiparticle weights for adding or removing an electron on the Fermi surface both converge to the value derived from the jump of the momentum distribution function on the Fermi surface, a result consistent with the Landau Fermi liquid theory. We also find the quasiparticle weights for adding or removing an electron vanish at half-filling, as predicted by the slave–boson mean-field theory. However, we do find that the quasiparticle weights calculated from the Gutzwiller projected wavefunction show modest particle–hole asymmetry at finite excitation energy, which becomes more evident near half-filling. Our calculation shows that the tunnelling asymmetry near the chemical potential should be attributed to the incoherent part of the electron spectrum. We propose to use the tunnelling asymmetry to study the mechanism of electron incoherence in the high-temperature superconductors.

In the Landau theory of a Fermi liquid, a quasiparticle plays a dual role. When exactly on the Fermi surface, a quasiparticle can be viewed either as a particle-like (or hole-like) elementary excitation on the ground state of an N-particle system, or a constituent particle (or hole) of the ground state of an $N + 1$ ($N - 1$)-particle system. Thus, the quasiparticle weight for adding an electron into the system on the Fermi surface is equal to the square of the matrix element of the electron creation operator between the ground state of an N-particle system and the ground state of an $N + 1$-particle system:

$$Z_N^+ = |\langle g_{N+1}|c_k^\dagger|g_N\rangle|^2,$$

while the quasiparticle weight for removing an electron from the system on the Fermi surface is equal to the square of the matrix element of electron annihilation operator between the ground state of an N-particle system and the ground state of an $N - 1$-particle system:

$$Z_N^- = |\langle g_{N-1}|c_k|g_N\rangle|^2 = Z_{N-1}^+.$$

In the thermodynamic limit, we have

$$Z_N^- = Z_{N-1}^+ \simeq Z_N^+.$$

Thus the quasiparticle weight should be particle–hole symmetric on the Fermi surface. This simple argument does not apply to the superconducting state. However, we do not expect the superconducting pairing to change the conclusion since the superconducting pairing is expected to enhance rather than reduce the particle–hole symmetry.

2. The Gutzwiller wavefunctions for the quasiparticles

Now we calculate the quasiparticle weight from the Gutzwiller projected wavefunctions. Such a variational description is widely used in the study of the t–J model and is believed to be able to capture the low-energy physics of the cuprate superconductors quite well [8–11]. The variational ground state, namely the Gutzwiller projected BCS state with N particles, is given by (we follow the notations used in [5])

$$|\Psi_0^N\rangle = P_N P_G|\text{BCS}\rangle, \tag{1}$$

where P_N is the projection operator into the subspace of N electrons, and $P_G = \prod_i (1-n_{i\uparrow}n_{i\downarrow})$ is the projection operator into the subspace of no double occupancy. $|\text{BCS}\rangle$ denotes the unprojected BCS mean-field ground state. The quasiparticle excitations above the variational ground state can be similarly constructed by Gutzwiller projection of BCS mean-field excited states. For example, a particle-like quasiparticle with momentum k and spin σ can be constructed as follows:

$$|\Psi_{k,\sigma}^{N+1}\rangle = P_{N+1} P_G \gamma_{k,\sigma}^\dagger|\text{BCS}\rangle, \tag{2}$$

where P_{N+1} is the projection operator into the subspace of $N + 1$ electrons and $\gamma_{k,\sigma}^\dagger$ is the creation operator for a Bogliubov quasiparticle on the BCS mean-field ground state. $\gamma_{k,\sigma}^\dagger$ is related to the original electron operator $c_{k,\sigma}^\dagger$ through the Bogliubov transformation:

$$\begin{pmatrix} \gamma_{k,\uparrow} \\ \gamma_{-k,\downarrow}^\dagger \end{pmatrix} = \begin{pmatrix} u_k & -v_k \\ v_k & u_k \end{pmatrix} \begin{pmatrix} c_{k,\uparrow} \\ c_{-k,\downarrow}^\dagger \end{pmatrix}, \tag{3}$$

in which $u_k = \sqrt{1 + \frac{\xi_k}{E_k}}$, $v_k = \sqrt{1 - \frac{\xi_k}{E_k}}$. Here ξ_k denotes the bare dispersion and $E_k = \sqrt{\xi_k^2 + \Delta_k^2}$ denotes the energy of the Bogliubov quasiparticle. Similarly, a hole-like quasiparticle with momentum k and spin σ can be constructed as follows:

$$|\Psi_{k,\sigma}^{N-1}\rangle = P_{\text{N}-1} P_G \gamma_{k,\sigma}^\dagger|\text{BCS}\rangle, \tag{4}$$

where $P_{\mathrm{N}-1}$ is the projection operator into the subspace of $N-1$ electrons. The quasiparticle weight for adding an electron is given by the overlap between the bare electronic state, namely $c^\dagger_{k,\sigma}|\Psi^N_0\rangle$, and the quasiparticle state $|\Psi^{N+1}_{k,\sigma}\rangle$, with proper normalization factor added:

$$Z^+_k = \frac{|\langle\Psi^{N+1}_{k,\sigma}|c^\dagger_{k,\sigma}|\Psi^N_0\rangle|^2}{\langle\Psi^{N+1}_{k,\sigma}|\Psi^{N+1}_{k,\sigma}\rangle\langle\Psi^N_0|\Psi^N_0\rangle}, \tag{5}$$

while the quasiparticle weight for removing an electron from the system is given by the overlap between $c_{-\mathrm{k},-\sigma}|\Psi^N_0\rangle$ and $|\Psi^{N-1}_{k,\sigma}\rangle$, with proper normalization factor added:

$$Z^-_k = \frac{|\langle\Psi^{\mathrm{N}-1}_{k,\sigma}|c_{-\mathrm{k},-\sigma}|\Psi^N_0\rangle|^2}{\langle\Psi^{\mathrm{N}-1}_{k,\sigma}|\Psi^{\mathrm{N}-1}_{k,\sigma}\rangle\langle\Psi^N_0|\Psi^N_0\rangle}. \tag{6}$$

As pointed out by Yunoki, using the fact that $P_G c^\dagger_{k,\sigma} P_G = P_G c^\dagger_{k,\sigma}$ [3], the quasiparticle weight for adding an electron with spin σ can be related to the momentum distribution function $n_k = \frac{1}{2}\sum_\sigma \langle c^\dagger_{k,\sigma} c_{k,\sigma}\rangle$ as follows:

$$Z^+_k = |u_k|^2 \frac{\langle\Psi^{N+1}_{k,\sigma}|\Psi^{N+1}_{k,\sigma}\rangle}{\langle\Psi^N_0|\Psi^N_0\rangle} = 1 - \frac{N_{\bar\sigma}}{L} - n_k, \tag{7}$$

where $N_{\bar\sigma}$ denotes the total number of electrons with the opposite spin, and L denotes the number of lattice sites. Thus to calculate Z^+_k, we only need to evaluate a ground-state expectation value. The calculation of Z^-_k is more complex. However, using the identity $P_G c^\dagger_{k,\sigma} P_G = P_G c^\dagger_{k,\sigma}$ and the Bogliubov transformation, we are able to show that

$$Z^-_k = f\frac{|u_k(v_k - u_k O_k)|^2}{\tilde{Z}^+_k}, \tag{8}$$

in which f is momentum independent and is given by

$$f = \frac{\langle\Psi^N_0|\Psi^N_0\rangle}{\langle\Psi^{\mathrm{N}-2}_0|\Psi^{\mathrm{N}-2}_0\rangle}, \tag{9}$$

and $\tilde{Z}^+_k$ denotes the quasiparticle weight for adding an electron in the ground state of an $N-2$ particle system, namely $|\Psi^{\mathrm{N}-2}_0\rangle$. O_k is a overlap integral and is given by

$$O_k = \frac{\langle\Psi^N_0|\Psi^N_{2k}\rangle}{\langle\Psi^N_0|\Psi^N_0\rangle}, \tag{10}$$

in which

$$|\Psi^N_{2k}\rangle = P_N P_G \gamma^\dagger_{k,\uparrow}\gamma^\dagger_{-\mathrm{k},\downarrow}|\mathrm{BCS}\rangle \tag{11}$$

denotes a state with a pair of quasiparticles. Now the calculation of Z^-_k is reduced to the calculation of $\tilde{Z}^+_k$, O_k, and the constant f. Technically, the calculations of $\tilde{Z}^+_k$ and O_k are much easier than the calculation of Z^-_k from its defining equation (6). To calculate Z^-_k directly from equation (6), one has to sample $|\Psi^{N-1}_{k,\sigma}\rangle$ for each individual momentum k. However, to calculate $\tilde{Z}^+_k$ and O_k, one only needs to sample a single wavefunction.

Further simplification is possible when there is no superconducting pairing. In such a case, one finds

$$Z^+_k = \frac{\langle\Psi^{N+1}_{k,\sigma}|\Psi^{N+1}_{k,\sigma}\rangle}{\langle\Psi^N_0|\Psi^N_0\rangle} \tag{12}$$

for k outside the Fermi surface and

$$Z^-_k = \frac{\langle\Psi^N_0|\Psi^N_0\rangle}{\langle\Psi^{\mathrm{N}-1}_{k,\sigma}|\Psi^{\mathrm{N}-1}_{k,\sigma}\rangle} \tag{13}$$

for k inside the Fermi surface. Noting the fact that $|\Psi_{k,\sigma}^{N+1}\rangle$ ($|\Psi_{k,\sigma}^{\mathrm{N}-1}\rangle$) is nothing but the variational ground state of the $N+1(N-1)$-particle system for k on the Fermi surface, we have

$$Z^{+}_{\mathrm{k}_\mathrm{F}^{+}} = \frac{\langle\Psi_0^{N+1}|\Psi_0^{N+1}\rangle}{\langle\Psi_0^{N}|\Psi_0^{N}\rangle} \tag{14}$$

and

$$Z^{-}_{\mathrm{k}_\mathrm{F}^{-}} = \frac{\langle\Psi_0^{N}|\Psi_0^{N}\rangle}{\langle\Psi_0^{\mathrm{N}-1}|\Psi_0^{\mathrm{N}-1}\rangle}, \tag{15}$$

where $k_\mathrm{F}^{\pm}$ denotes momentum just above or below the Fermi surface. Thus, if the quasiparticle weight is a continuous function of particle number, it should be particle–hole symmetric on the Fermi surface in the thermodynamic limit. Furthermore, using Yunoki's relation and the fact that Z_k^{+} vanishes for k inside the Fermi surface, we have

$$n_k = 1 - \frac{n}{2} \tag{16}$$

for k inside the Fermi surface and

$$Z^{+}_{\mathrm{k}_\mathrm{F}^{+}} = \Delta n_{\mathrm{k}_\mathrm{F}}, \tag{17}$$

where $\Delta n_{\mathrm{k}_\mathrm{F}}$ denotes the jump of n_k on the Fermi surface. Thus both Z_k^{+} and Z_k^{-} converge to $\Delta n_{\mathrm{k}_\mathrm{F}}$ on the Fermi surface in the thermodynamic limit, a result consistent with the standard Fermi liquid theory.

3. Method

The calculation of the quasiparticle weight is now reduced to the calculation of the quantities of the form $\frac{\langle\Psi_1|\hat{O}|\Psi_2\rangle}{\langle\Psi_1|\Psi_1\rangle}$, where $\hat{O}$ denotes a general physical operator. These quantities can be calculated easily by the standard variational Monte Carlo method. First, we expand both $|\Psi_1\rangle$ and $|\Psi_2\rangle$ in the Fock basis $|\alpha\rangle = \prod_{i_\alpha, j_\alpha} c^{\dagger}_{i_\alpha\uparrow} c^{\dagger}_{j_\alpha\downarrow}|0\rangle$, with $\psi_{1\alpha}$ and $\psi_{2\alpha}$ as their amplitudes. Here i_α and j_α denote the sets of spatial coordinates of the up-spin electrons and the down-spin electrons in the given configuration $|\alpha\rangle$. For the wavefunctions considered in this paper, the amplitudes in the Fock basis are Slater determinants of matrices composed of the eigenfunctions of the single-particle Hamiltonian equations (19) and (20). The quantity to be calculated is now reduced to

$$\frac{\langle\Psi_1|\hat{O}|\Psi_2\rangle}{\langle\Psi_1|\Psi_1\rangle} = \frac{\sum_\alpha |\psi_{1\alpha}|^2 \frac{\sum_\beta O_{\alpha\beta}\psi_{2\beta}}{\psi_{1\alpha}}}{\sum_\alpha |\psi_{1\alpha}|^2}, \tag{18}$$

where $O_{\alpha\beta} = \langle\alpha|\hat{O}|\beta\rangle$ denotes the matrix element of $\hat{O}$ in the Fock basis. To calculate the weighted sum in equation (18), one follows the standard Metropolis procedure to generate a series of sample configurations $|\alpha_1\rangle, \ldots, |\alpha_M\rangle$ distributed according to the probability $|\psi_{1\alpha}|^2$. The quantity to be calculated is then approximated by the average of $\frac{\sum_\beta O_{\alpha\beta}\psi_{2\beta}}{\psi_{1\alpha}}$ over the M generated Monte Carlo samples. A more detailed explanation of the method can be found in the review by Gros [14].

In our calculation, we have used 500 000 samples in each case to estimate the quantity to be evaluated. Since there is no systematic error in the calculation, the accuracy of the results can be read off from the smoothness of the curves obtained. To give an absolute measure of the statistical error in our calculation, we note that the fluctuation in the energy of the t–J model calculated with the wavefunctions in this paper is less than $10^{-4}t$ on a 18×18 lattice. With such an accuracy one is able to derive a rather smooth dispersion relation for the quasiparticle.

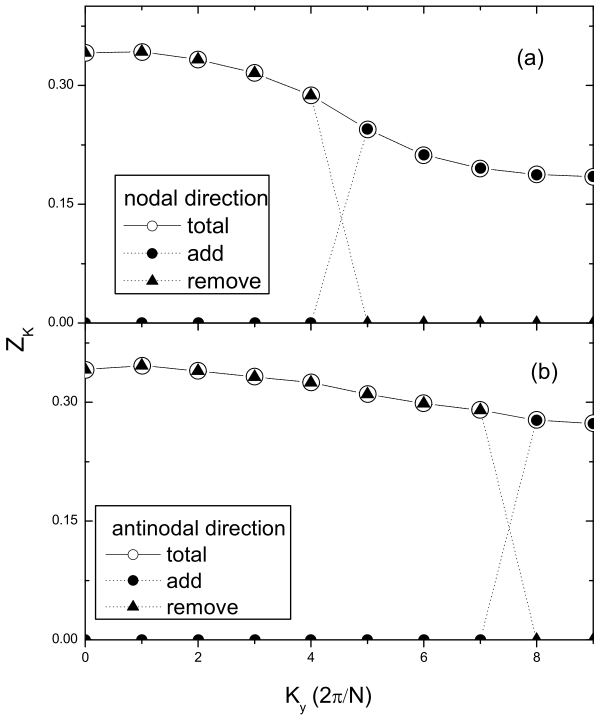

Figure 1. The quasiparticle weight as calculated from the VMC method for a Gutzwiller projected Fermi sea state on an 18×18 square lattice with 42 holes ($x \simeq 0.13$). The hole number is so chosen that the closed shell condition is satisfied for a system with periodic–periodic boundary condition. The mean-field state is generated by the mean-field Hamiltonian equation (18). (a) Quasiparticle weight in the $(0, 0)$–(π, π) (nodal) direction. (b) Quasiparticle weight in the $(0, 0)$–$(0, \pi)$ (antinodal) direction.

4. Results

We now present the results of the VMC calculation. Figure 1 shows the quasiparticle weight evaluated on a Gutzwiller projected Fermi sea state. The Gutzwiller projected Fermi sea state is generated by the following mean-field Hamiltonian:

$$H_{\mathrm{MF}} = -\sum_{\langle ij\rangle,\sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + \mathrm{h.c.}) - \mu \sum_{i\sigma} c^{\dagger}_{i\sigma} c_{i\sigma}, \quad (19)$$

in which $\sum_{\langle ij\rangle}$ denotes the sum over nearest-neighbouring sites on the square lattice. The ground state of this Hamiltonian is a Fermi sea state,

$$|\mathrm{FS}\rangle = \prod_{k<\mathrm{k_F}} c^{\dagger}_{k\uparrow} c^{\dagger}_{k\downarrow} |0\rangle, \quad (20)$$

where $c^{\dagger}_{k\uparrow}$ is the creation operator of an electron with momentum k and an up spin, k_{F} is the Fermi momentum determined by the electron filling, and $|0\rangle$ denotes the vacuum of an electron. The Gutzwiller projected Fermi sea state is generated from $|\mathrm{FS}\rangle$ by removing its components with doubly occupied sites.

The results are shown for two representative directions in the Brillouin zone: the $(0, 0)$–(π, π) direction and the $(0, 0)$–$(\pi, 0)$ direction. Below the Fermi surface, the quasiparticle weight for adding an electron is zero, while above the Fermi surface, the

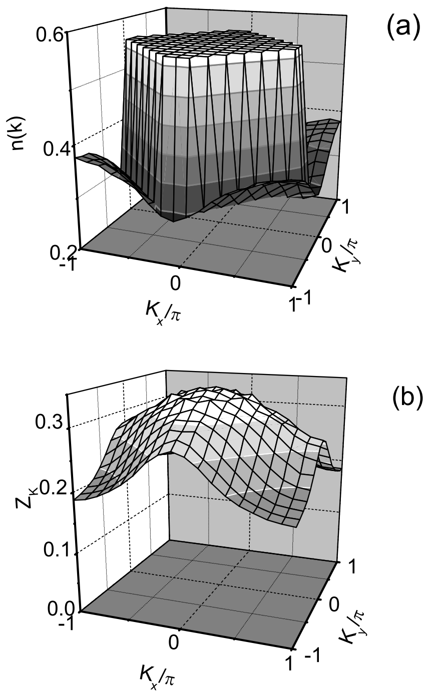

Figure 2. The momentum distribution function (a) and the total quasiparticle weight (b) of the Gutzwiller projected Fermi sea state as calculated from the VMC method in the whole Brillouin zone. The parameters used in the calculation are the same as those of figure 1.

quasiparticle weight for removing an electron is zero. Thus, both Z_k^+ and Z_k^- show a jump on the Fermi surface. However, we find that the total quasiparticle weight, namely $Z_k^+ + Z_k^-$, is a continuous function of momentum across the Fermi surface. This can be seen more clearly in figure 2(b), in which the total quasiparticle weight is plotted in the whole Brillouin zone. The continuity of the total quasiparticle weight implies that the quasiparticle weight should be particle–hole symmetric on the Fermi surface in the thermodynamic limit, as we have argued above.

Away from the Fermi surface, the calculated quasiparticle weight shows modest particle–hole asymmetry at the doping level considered ($x \simeq 0.13$). The quasiparticle weight for removing an electron is larger than that for adding an electron. In general, the total quasiparticle weight decreases monotonically with momentum in all radial directions from $(0, 0)$ in the Brillouin zone. As can be seen from equation (7), the momentum dependence of Z_k^+ can be understood from that of $n(k)$. The calculated $n(k)$ for the Gutzwiller projected Fermi sea state is shown in figure 2(a). Below the Fermi surface, $n(k)$ is a constant. Above the Fermi surface, $n(k)$ is an *increasing* function of momentum in all radial directions from $(0, 0)$ in the Brillouin zone. This rather unusual behaviour is characteristic of the Gutzwiller-type projected wavefunctions, and results in the decrease of Z_k^+ above the Fermi surface. We note that the non-monotonic behaviour of $n(k)$ is related to the correlated nature of the hopping term in the t–J model [12] and is not an artefact of the Gutzwiller projected wavefunctions[5].

[5] The momentum distribution function of the t–J model differs from the that of the Hubbard model by a canonical transformation. The momentum distribution function after the canonical transformation is a monotonic function of momentum.

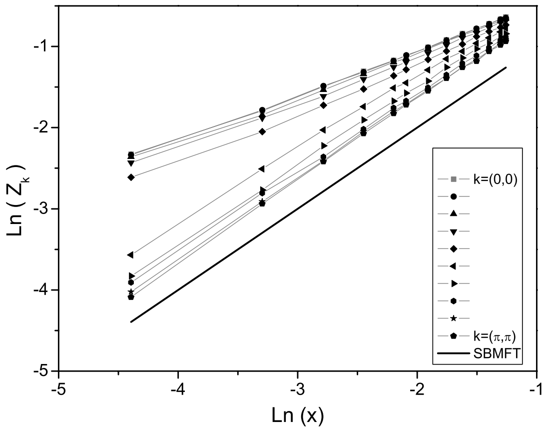

Figure 3. Doping dependence of the quasiparticle weight as calculated from the VMC method for the Gutzwiller projected Fermi sea state. The calculation is done on an 18×18 lattice with periodic–antiperiodic boundary condition. Shown in the figure are the results for the ten momenta along the $(0,0)$–(π,π) direction. Among the ten curves in the figure, the upper five are for momenta below the Fermi surface and the lower five are for momenta above the Fermi surface at sufficiently low doping (at higher doping level, a momentum originally below the Fermi surface can be transformed into a momentum above the Fermi surface with increasing doping). Also shown in the figure (as a bold solid line) is the prediction of the slave–boson mean-field theory (SBMFT).

The doping dependence of the quasiparticle weight is shown in figure 3. Plotted in the figure is the result for all the ten momenta in the $(0,0)$–(π,π) direction of an 18×18 lattice. The quasiparticle weight predicted by the slave–boson mean-field theory (which is momentum independent) is also shown in the figure for comparison. From the figure we see that the quasiparticle weights for adding and removing an electron from the system both vanish near half-filling. According to the sum rule, the local spectral weight (which is given by the mean value of the spectral weight in the Brillouin zone) for removing an electron with a given spin is $\frac{1-x}{2}$, while that for adding an electron is x. Thus at sufficiently low doping level, most of the spectral weight in the hole side of the electron spectrum should be incoherent. Since the particle side of the electron spectrum only contains the coherent (or quasiparticle) contribution, the tunnelling asymmetry should be attributed to the incoherent spectral weight at sufficiently low doping level. Another interesting feature of figure 3 is that the quasiparticle weight for removing an electron decreases more slowly than that for adding an electron does. At the same time, the quasiparticle weight calculated from the Gutzwiller projected wavefunction is larger than that predicted by the SBMFT. These points will be discussed in more detail below.

Now let us compare our results with the predictions of other theories. In the slave–boson mean-field theory, the quasiparticle weight is reduced from the non-interacting value by a constant factor x (the hole density) but will still be particle–hole symmetric: $Z_k^+ = xu_k^2$ and $Z_k^- = xv_k^2$. At the same time, the SBMFT predicts that the electron spectrum in the particle side is totally coherent, while that in the hole side contains both coherent and incoherent contributions. Thus, one should attribute the tunnelling asymmetry totally to the incoherent spectral weight, which dominates the electron spectrum at sufficiently low doping level. The quasiparticle weight calculated from the Gutzwiller projected wavefunction agrees with the SBMFT prediction in two aspects. First, the quasiparticle weights for adding and removing an electron both vanish near half-filling. Second, the particle side of the electron spectrum is exhausted by the quasiparticle contribution. This implies that the tunnelling asymmetry should be attributed to the incoherent part of the electron spectrum at sufficiently low doping level, a conclusion in agreement with the prediction of the SBMFT.

However, unlike the prediction of the SBMFT, the quasiparticle weight calculated from the Gutzwiller projected wavefunction is particle–hole symmetric only near the Fermi surface, rather than symmetric in the whole Brillouin zone. In particular, in the absence of superconducting pairing, the quasiparticle weight predicted by the SBMFT reduces to a constant x, while the quasiparticle weight calculated from the Gutzwiller projected wavefunction is momentum dependent. As we have seen above, the calculated quasiparticle weight for removing an electron is always larger than that for adding an electron. The difference in the doping dependence of the quasiparticle weight predicted by these two approaches is even more dramatic. In the slave–boson mean-field theory, the quasiparticle weight scales linearly with x at all momenta. On the other hand, the quasiparticle weights calculated from the Gutzwiller projected wavefunction scale with x in different ways in the particle side and the hole side of the electron spectrum (see figure 3). More specifically, we find that the quasiparticle weight for adding an electron scales linearly with x at sufficiently low doping. However, the quasiparticle weight for removing an electron from the system follows approximately the $\sqrt{x}$ rule near half-filling. Thus the particle–hole asymmetry in the quasiparticle weight becomes more evident in relative terms with decreasing doping [7]. We note that the particle–hole asymmetry in the quasiparticle weight calculated from the Gutzwiller projected wavefunctions can be understood as a result of recombination of slave particles in the SBMFT [13].

As we have mentioned above, the quasiparticle weight calculated from the Gutzwiller projected wavefunction is larger than that predicted by the SBMFT. In the hole side of the electron spectrum, such a difference can be understood as a result of the recombination of slave particles in the SBMFT. In the particle side of the electron spectrum, in which the spectral weight is exhausted by the quasiparticle contribution in both the SBMFT and the Gutzwiller projected wavefunction approach, such a difference can be understood in terms of the sum rule. In the SBMFT theory, the local spectral weight (which is given by the mean value of the spectral weight in the Brillouin zone) for removing an electron with a given spin is $\frac{1-x^2}{2}$, while that for adding an electron is $\frac{x(1+x)}{2}$.[6] Thus for small x, the average of Z_k^+ predicted by SBMFT is about one half of that calculated from the Gutzwiller projected wavefunction. We note that the total local spectral weight predicted by the SBMFT is still the correct value $\frac{1+x}{2}$ for electron with a given spin.

Recently, Anderson and Ong calculated the quasiparticle weight of the Gutzwiller projected wavefunction and arrived at a conclusion quite different from ours [3]. They found that both the particle side and the hole side of the electron spectrum are dominated by the quasiparticle contribution for all doping levels. According to their calculation, there will be a jump in the total quasiparticle weight right at the Fermi surface when there is no superconducting paring. They argued that the tunnelling asymmetry observed in the STM experiments should be attributed to the coherent rather than incoherent part of the electron spectrum. These differences can be attributed to the approximation used in their calculation. They used the Gutzwiller approximation to treat the projection operator, while no approximation is used in our calculation. This indicates that the Gutzwiller approximation, which is useful for the estimation of ground-state expectation values, cannot be applied without change to the study of the quasiparticle excitation above the ground state. The approximation overestimates the coherent nature of the electron spectrum.

[6] In the SBMFT, the quasiparticle weight for adding an electron is a constant x above the Fermi surface and zero below the Fermi surface. Thus the average of Z_k^+ in the Brillouin zone is given by $\frac{x(1+x)}{2}$. Here we have used the fact that $\frac{1+x}{2}$ of the Brillouin zone is left unoccupied at hole density x.

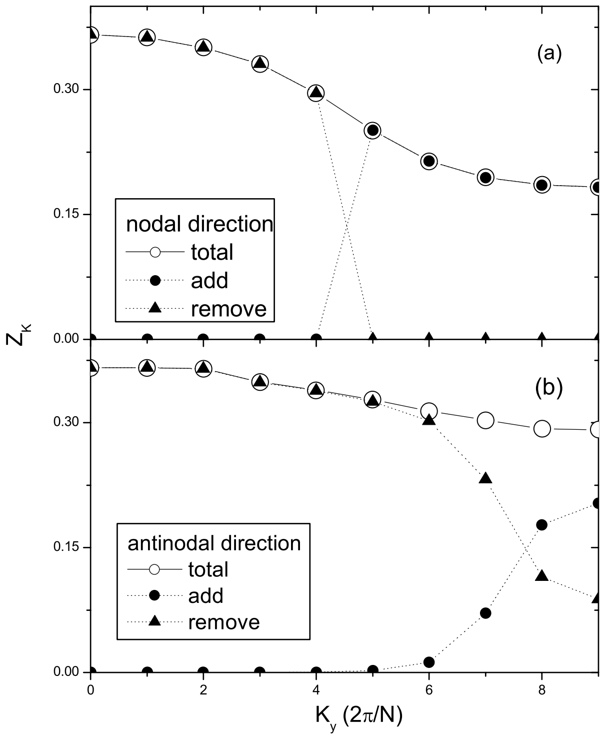

Figure 4. VMC results for the Gutzwiller projected d-wave BCS state. The calculation is done on an 18×18 lattice with 42 holes. $\frac{\Delta}{t} = 0.1$ and μ is determined by the mean-field equation for the electron density. (a) Quasiparticle weight in the $(0, 0)$–(π, π) (nodal) direction. (b) Quasiparticle weight in the $(0, 0)$–$(0, \pi)$ (antinodal) direction.

We now present the results for the Gutzwiller projected d-wave BCS state, which is believed to be a good approximation for the superconducting state of the high-T_c superconductors. The mean-field state to be projected is generated by the following BCS mean-field Hamiltonian:

$$H_{\mathrm{MF}} = -\sum_{\langle ij\rangle,\sigma}(c_{i\sigma}^{\dagger}c_{j\sigma} + \mathrm{h.c.}) - \mu\sum_{i\sigma}c_{i\sigma}^{\dagger}c_{i\sigma} + \Delta\sum_{\langle ij\rangle}d_{ij}(c_{i\uparrow}^{\dagger}c_{j\downarrow}^{\dagger} + c_{j\uparrow}^{\dagger}c_{i\downarrow}^{\dagger} + \mathrm{h.c.}), \tag{21}$$

in which d_{ij} is the form factor for d-wave pairing on the square lattice and the sum is over pairs of nearest-neighbouring sites. The mean-field ground state of this Hamiltonian takes the standard BCS form

$$|\mathrm{BCS}\rangle = \prod_k (u_k + v_k c_{k\uparrow}^{\dagger}c_{-\mathrm{k}\downarrow}^{\dagger})|0\rangle, \tag{22}$$

in which $u_k = \sqrt{1+\frac{\xi_k}{E_k}}$, $v_k = \sqrt{1-\frac{\xi_k}{E_k}}$. Here $\xi_k = -2(\cos k_x + \cos k_y) - \mu$, $E_k = \sqrt{\xi_k^2 + \Delta_k^2}$, $\Delta_k = 2\Delta(\cos k_x - \cos k_y)$.

The calculated quasiparticle weight is shown in figure 4 for momenta in the $(0, 0)$–(π, π) direction and the $(0, 0)$–$(0, \pi)$ direction. The results are similar to those shown in figure 1 for the projected Fermi sea state, except for the particle–hole mixture in the vicinity of the Fermi surface in the antinodal direction. Figure 5 shows the momentum dependence of the momentum distribution function $n(k)$ and the total quasiparticle weight $Z_k^+ + Z_k^-$ in the whole Brillouin zone. Again, the results are similar to those shown in figure 2 for the projected Fermi sea state.

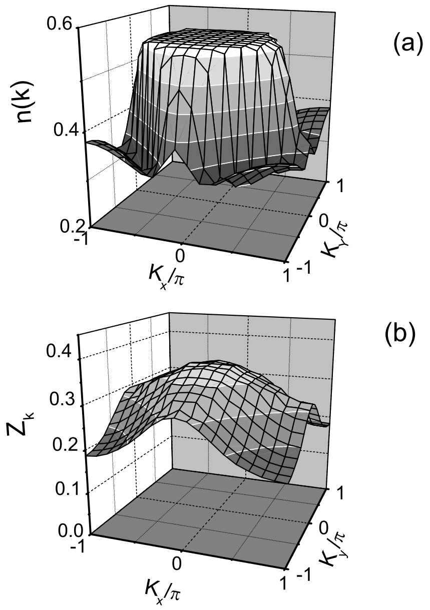

Figure 5. The momentum distribution function (a) and the total quasiparticle weight (b) of the Gutzwiller projected d-wave BCS state. The parameters used in the calculation are the same as those of figure 4.

Thus, the existence of superconducting pairing does not change our conclusions qualitatively, only making the momentum distribution function more rounded near the Fermi surface and causing some particle–hole mixture in the same momentum region.

Recently, it is found that the quasiparticle weight for adding an electron into the Gutzwiller projected d-wave BCS state exhibits an interesting pocket structure around the nodal point of the d-wave gap [6]. We find that such a pocket structure is absent in the total quasiparticle weight, which is found to be a monotonic decreasing function of momentum in all radial directions from (0, 0). To clarify the situation, we plot in figure 6 the momentum dependence of Z_k^+ and Z_k^- separately in the Brillouin zone. As shown in the figure, Z_k^+ is a non-monotonic function of momentum and it exhibits well-defined pocket structure around the nodal point of the d-wave gap. More specifically, in the radial direction from (0, 0), Z_k^+ is an increasing function of momentum below a momentum near the Fermi surface, but then it decreases with further increase of momentum. On the other hand, Z_k^- is a monotonic function of momentum in all radial directions from (0, 0) and the pocket structure found in Z_k^+ is totally absent.

The pocket structure in Z_k^+ can be understood in terms of the momentum dependence of $n(k)$. According to equation (7), the pocket in Z_k^+ corresponds to a similar pocket structure in $n(k)$ around the nodal point of the d-wave gap. The pocket structure in $n(k)$ can be understood as follows. For momentum much below the Fermi surface, $n(k)$ is a decreasing function of momentum in the radial direction from (0, 0), as the particle–hole mixing caused by pairing decreases with the distance from the Fermi surface, while for momentum much above the Fermi surface, $n(k)$ becomes an increasing function of momentum as a result of the intrinsic momentum dependence of $n(k)$ in the Gutzwiller projected Fermi sea state. Thus, $n(k)$ should be a non-monotonic function of momentum in any chosen radial direction from (0, 0) and will reach its minimum in that direction at some momentum near the Fermi surface. As the chosen direction of momentum rotates from the nodal direction to the antinodal direction, the minimal value of $n(k)$ that can be reached will also increase as a result of the increase of

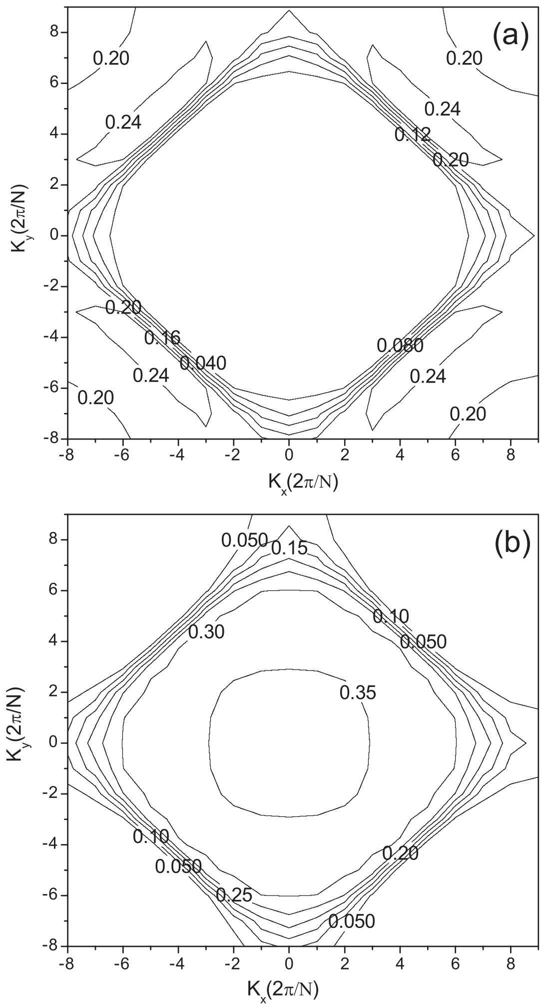

Figure 6. Momentum dependence of Z_k^+ (a) and Z_k^- (b) in the Gutzwiller projected d-wave BCS state.

the particle–hole mixing and the smearing of the Fermi surface singularity. Combining these reasonings, one concludes that there should be a pocket structure in $n(k)$ around the nodal point. Since the increase of $n(k)$ above the Fermi surface (which makes $n(k)$ non-monotonic in the radial direction from $(0, 0)$) is an intrinsic property of the t–J model and also of the Gutzwiller projected wavefunction, we think that the pocket structure in Z_k^+ should be a generic feature of the Gutzwiller projected wavefunction with a d-wave-type pairing gap. For Z_k^-, the above reasoning does not apply. Now there is no understanding on the origin of its momentum dependence. However, since it is a monotonic function of momentum in all radial direction from (0, 0), there can be no pocket structure in Z_k^-. The same is true for the total quasiparticle weight $Z_k^+ + Z_k^-$.

5. Conclusion

In summary, we have shown that the quasiparticle weight calculated from the Gutzwiller projected wavefunction for the cuprate superconductors is particle–hole symmetric at sufficiently low energy. At the same time, we have shown that the quasiparticle weight in both the particle and the hole side of the electron spectrum vanishes at half-filling, which indicates that the electron spectrum is dominated by the incoherent spectral weight at sufficiently low doping level. Since the incoherent spectral weight is proved to be totally absent in the particle side of the electron spectrum, we should attribute the majority of the observed tunnelling asymmetry to the incoherent part of the electron spectrum. These results agree qualitatively with the predictions of the SBMFT, but disagree with that of a Gutzwiller approximation on the projected wavefunction. However, we have found that the quasiparticle weight calculated from the Gutzwiller projected wavefunction does show modest particle–hole asymmetry at finite bias, which becomes more evident in relative terms with decreasing doping. This asymmetry is shown to be related to the difference in the doping dependence of the particle-like and the hole-like quasiparticle weight. Both the SBMFT and the Gutzwiller approximation are not able to predict the correct behaviour of the quasiparticle weight as a function of momentum and doping. We have found that the pocket structure in Z_k^+ noticed in a previous study should be a generic feature of the Gutzwiller projected wavefunctions with d-wave pairing gap. However, no corresponding pocket exists in Z_k^- or $Z_k^+ + Z_k^-$.

From our calculation, we see that the quasiparticle behaviour predicted by the Gutzwiller projected wavefunction follows the canonical Fermi liquid theory near the Fermi surface. Thus, if we take the Gutzwiller projected d-wave BCS state as a reasonable description of the superconducting state of the high-T_c superconductors, the quasiparticle excitation above such a strongly correlated state should still be described by the standard Fermi liquid theory. Our calculation also indicates that at sufficiently low doping level the electron spectrum is dominated by the incoherent spectral weight. This is in agreement with the experimental findings from ARPES measurements [15]. Thus, a full description of the low-energy physics of the system should also include these incoherent spectral weight.

Acknowledgments

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