PSEUDO GAPS AND SPIN BAGS

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It is shown that antiferromagnetic spin fluctuations in a two-dimensional metal, such as heavily doped cuprate superconductors, lead to a pseudo gap in the electronic spectrum. The self-energy of spin bags and their pairing interaction in the paramagnetic metal are calculated. These results are consistent with the corresponding results in the weakly doped ordered antiferromagnet.

1. Introduction

The existence of antiferromagnetism and superconductivity in nearby regions of the phase diagram of cuprates, as shown in fig. 1, suggests that local spin order plays an important role in bringing about superconductivity at high temperature. Finite range antiferromagnetic spin correlations are observed for doping concentrations in the superconducting range and larger [1], with these correlations eventually vanishing in the strongly doped metallic phase.

It was proposed [2] that bag-like excitations exist in both the paramagnetic metal and antiferromagnetic phases, in which there is a pseudo gap or actual gap for adding a carrier. These spin bags correspond to a local reduction of spin order in the vicinity of an added hole (or electron for the n type doped materials). The spin bags attract by sharing each other's region of reduced spin order, or equivalently reduced gap energy.

This proposal was investigated in the antiferromagnetic phase by Wen, Zhang and one of the authors (SWZ) [3], who showed that the pairing interaction between spin bags is in fact attractive, in contrast to the one fluctuation repulsion between quasi particles occurring in the strongly metallic phase [4].

In this paper, we discuss the problem starting from the large doping limit for which the material is a good paramagnetic metal rather than an antiferromagnetic insulator. We show that while the one particle self-energy is of the Fermi liquid form for large doping, as x is reduced, antiferromagnetic spin fluctuations grow in strength with a pseudo gap in the electronic spectrum gradually setting in for the doping level approaching the superconducting regime. In the pseudo gap regime, the one particle spectral weight function has two peaks rather than one as in the Fermi liquid regime.

The mechanism which brings about the pseudo gap can be seen by dividing the self-energy in the spin polaron Σ_{pol} and vacuum fluctuation Σ_{vf} parts. It is shown that the pseudo gap arises from the spin susceptibility peaking at the antiferromagnetic wave vector $\boldsymbol{Q}$. This causes the energy lowering due to polaron effects in the Fermi liquid to be sharply reduced while the Pauli principle suppression of vacuum fluctuations leads to an increase of energy, forming the pseudo gap. A spin bag corresponds to the decrease of the magnitude of the pseudo gap in a region of order of the spin coherence length surrounding the hole.

We show that the pairing interaction between spin bags in the paramagnetic regime is attractive for small

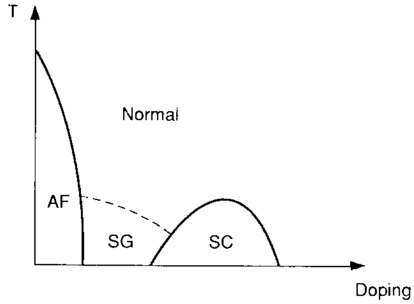

Fig. 1. A schematic phase diagram of the cuprate superconductors. AF, antiferromagnetic; SG, spin glass; SC, superconducting. x is the hole concentration.

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momentum transfer, as SWZ found in the spin ordered phase.

2. Self-energy

We consider the 2d one orbital Hubbard model on a square lattice. At half filling the nesting property of the Fermi surface is known to produce antiferromagnetic spin order, i.e., a spin density wave (SDW) of wave vector $Q = (\pi/a, \pi/a)$. For doping x larger than a critical value, x_c, spin order exists only over a finite range L_{ss}, with the spin susceptibility $\chi(q, \omega)$ exhibiting a peak around Q with a half width of order L_{ss}^{-1}.

To study how the onset of spin fluctuations affects the self-energy, we consider $\Sigma(k, \omega)$ in the onc loop approximation shown in fig. 2. If the injected carrier is a hole, the intermediate state in fig. 2a is an electron and in fig. 2b is a hole, while the reverse is true if an electron is injected. Thus, diagram 2b is the conventional polaron contribution to the self-energy Σ_{pol} and is negative near the Fermi surface. This term lowers the energy of the injected particle, building up the density of states at the Fermi surface.

On the other hand, the "backward propagation" diagram in fig. 2a has just the reverse effect, raising the energy of the injected carrier. The physical origin of this increase is simply that vacuum spin fluctuations which lower the system energy in the absence of the added carrier are suppressed by the exclusion principle, giving an overall energy increase, so that Σ_{vf} is positive.

Which of these two self-energy effects wins out depends on the form of the susceptibility $\chi(q, \omega)$. In the Fermi liquid regime, χ varies smoothly with q on the scale of the Fermi momentum. In this case Σ_{pol} dominates and the spectral function has one peak. As antiferromagnetic spin fluctuations build up, χ becomes peaked about the nesting wave vector $Q = (\pi/a, \pi/a)$. The essential point is that if an electron is injected in a state k above the Fermi momentum, the intermediate state $k + Q$ is necessarily below the Fermi surface. This is possible only if the intermediate state is a hole, as in fig. 2a. In this limit Σ_{pol} is small compared to Σ_{vf} and a pseudo gap is formed.

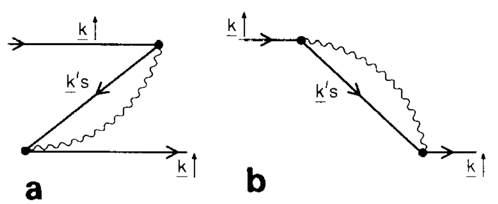

Fig. 2. "Backward" a) and "forward propagation" time-ordered Feynman diagram b). a) represents the contribution from the suppression of vacuum fluctuations and b) represents the spin-polaron contribution. s is up or down corresponding to the spin-flip or non spin-flip susceptibility, respectively.

To demonstrate this effect consider the simple model susceptibility [5]

$$\chi(q, \omega) = -\int d\omega' g(\omega') \frac{2\omega'\lambda^2}{\omega^2 - \omega'^2 + i\delta} \times \sum_{Q=(\pm\pi/a, \pm\pi/a)} \frac{\Gamma}{(q-Q)^2 + \Gamma^2} \tag{1}$$

which has the basic feature that it is enhanced around the nesting wave vectors $Q = (\pm\pi/a, \pm\pi/a)$. The static Lee–Rice–Anderson like model [6] is recovered for $g(\omega) = \lim_{\omega_0 \to 0} \delta(\omega - \omega_0)$. We consider, for example, a linear frequency distribution

$$g(\omega) = \frac{2}{\omega_0} \frac{\omega}{\omega_0} \theta(\omega_0 - \omega) . \tag{2}$$

Using this susceptibility, we evaluate the self-energy

$$\Sigma(k, \omega) = -\tfrac{3}{2} i U^2 \frac{1}{N} \sum_q \int \frac{d\nu}{2\pi} G(k - q, \omega - \nu) \times \chi(q, \nu) \tag{3a}$$

$$= \Sigma_{vf} + \Sigma_{pol} . \tag{3b}$$

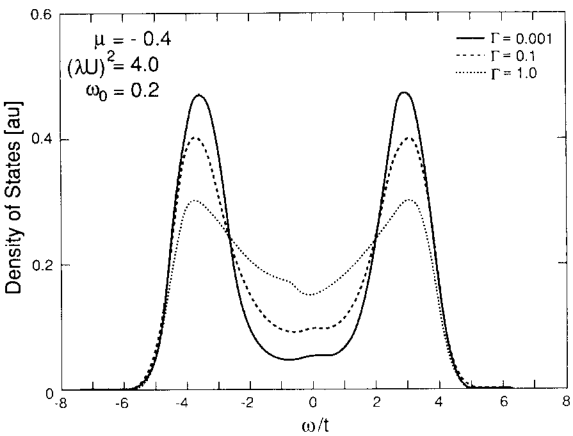

Fig. 3. Density of states as calculated from the model susceptibility for different values of Γ.

Γ^{-1} is a measure for the effective spin–spin correlation length measured in units of the lattice spacing. By varying Γ we can continuously cross over from the paramagnetic metal regime for $\Gamma \sim 1$ to the pseudo gap behavior for $\Gamma \ll 1$. The corresponding evolution of the density of states, calculated as the momentum space average of the spectral function

$$A_k(\omega) = \frac{1}{\pi} |\mathrm{Im}\, G(k, \omega + \mu)| \tag{4}$$

is shown in fig. 3. Similarly, the pseudo gap develops within the 2d single orbital Hubbard model away from half-filling by varying the Coulomb energy U or the hole doping concentration [5].

3. Pairing interaction

Based on the spin bag approach we have proposed an alternative pairing mechanism for high-T_c materials. As demonstrated above strong antiferromagnetic spin correlations lead to a pseudo gap in the quasi particle spectrum. The pairing attraction $V_{kk'}$ arises in this approach from the lowering of the system energy when two quasi particles share the region of reduced antiferromagnetic correlations surrounding each of these excitations. The range of this attraction is of order the SDW coherence length ξ_{SDW}. In momentum space, this corresponds to an attraction for momentum transfer q smaller than ξ_{SDW}^{-1}.

Contributions to the effective interaction between a pair of holes (or particles) can be obtained by accounting for the effects on the self-energy due to the presence of the second hole. Starting with the self-energy contribution in fig. 4a, the presence of a second particle with the same spin and momentum as the intermediate fermion line (not involving the bubbles) requires one to include the exchange graph fig. 4b in order to restore the Pauli principle. Stretching out the lines it is clear that this diagram is just the repulsive one spin fluctuation exchange process [7]. The corresponding diagram for particles of opposite spin involves an even number of bubbles. In addition, the spin-flip interaction corresponding to the particle–hole ladder must be added to preserve spin rotation invariance.

However, the existence of the pseudo gap does provide a new mechanism for an attractive spin bag pairing potential. It arises from the exclusion principle violation shown in fig. 5a, where a fermion line inside

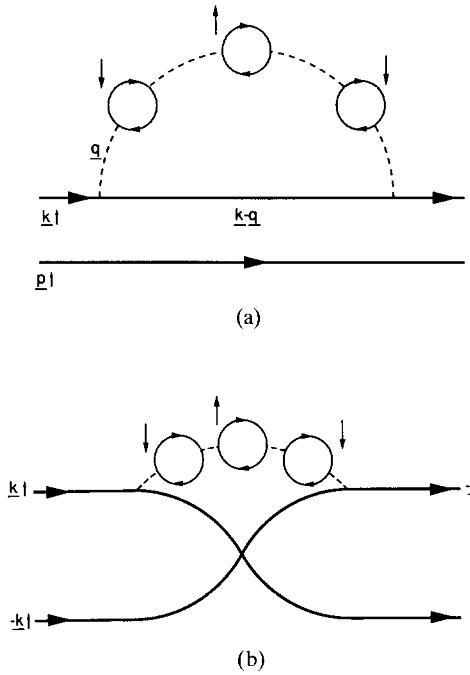

Fig. 4. Self-energy diagram in the presence of a second injected particle a); exchange diagram restoring the Pauli principle b).

one of the bubbles representing the susceptibility is equal to the momentum of the injected particle. This diagram is compensated by its exchange counterpart shown in fig. 5b, or the crossed line diagram shown in fig. 5c. The fact that this diagram leads to an attraction is readily seen. As discussed above, the self-energy due to spin flucutations is positive near the SDW instability and leads to a pseudo gap. A second particle added to the system suppresses these fluctuations through the Pauli principle, reducing the phase space for electron–hole excitations and hence reducing χ. This real space reduction of susceptibility extends over a range of order ξ_{SDW} around each quasiparticle and reduces the self-energy for another particle in its vicinity, thereby giving an effective attraction.

The effective pairing potential $V_{\mathrm{eff}}(k, k')$ is the sum of the attractive spin bag interaction $V_{\mathrm{SB}}(k, k')$ and the repulsive contribution from the antiparamagnon exchange processes $V_{\mathrm{APM}}(k, k')$. Since V_{SB} is largest for small $q = k - k'$ and V_{APM} is largest for large $q \simeq Q$, the effective pairing potential is attractive for small momentum transfer and repulsive for large momentum transfer [5]. This is the same behavior that

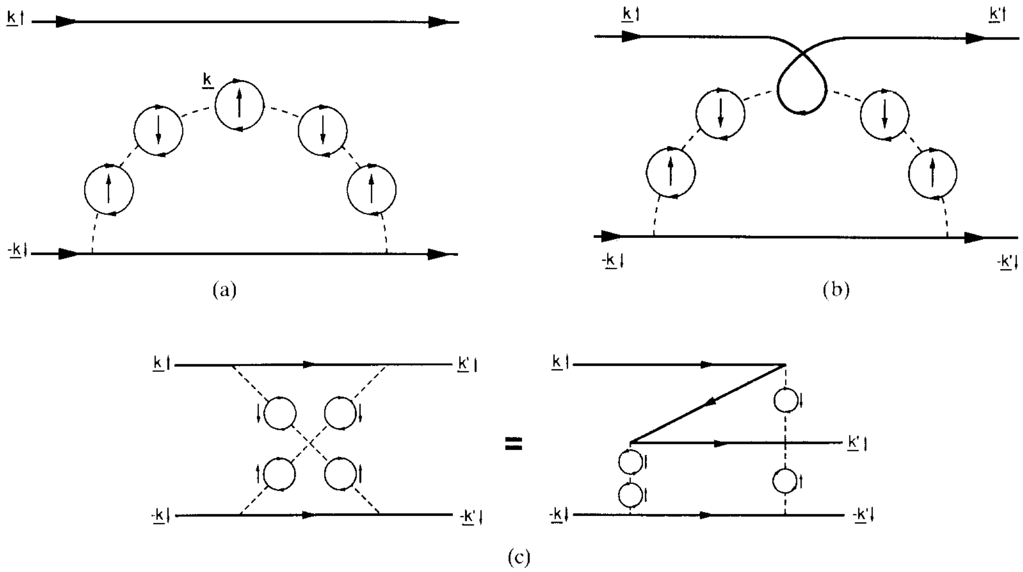

Fig. 5. Lowest order spin bag contribution to the pairing interaction.

SWZ [3] deduced for V_{eff} in the antiferromagnetic phase.

4. Conclusion

We have shown how antiferromagnetic spin fluctuations depress the density of states in the vicinity of the Fermi surface, leading to a pseudo gap. Injected particles reduce the amplitude of fluctuations and thereby reduce locally the size of the pseudo gap. This combination of a hole (electron) moving with its region of reduced antiferromagnetic correlations is termed a spin bag. We have shown that the pairing interaction between two spin bags is attractive for small momentum transfer due to the holes sharing each other's bag and repulsive for large momentum transfer reflecting the repulsive nature of the spin fluctuation exchange process. This repulsive feature of the pairing interaction suggests that the pairing gap parameter Δ_{SC} formally has d-wave like symmetry. However, if hole doping at the four corners of the magnetic zone leads to hole pockets which do not overlap due to the small density of states in the pseudo gap the system will appear to have a nodeless order parameter on the whole Fermi surface and to be very different from a conventional d-wave superconductor.

Acknowledgement

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