One-particle excitations in strong-coupling superconductors: A new realization of the t-J model

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We study the one-particle excitations in strong-coupling superconductors described by a negative-U Hubbard Hamiltonian. We show that the problem of single-particle excitation can be mapped onto that of a hole in a polarized antiferromagnetic Heisenberg model. We discuss—using a self-consistent diagrammatic approach—the distortion of the superfluid order parameter in the vicinity of the quasiparticle and the connection with the pairing-bag problem.

The discovery of high-T_c superconductors has renewed the interest in a number of old ideas and has also triggered the proposal of new unconventional ones. In the quest for the understanding of high-T_c superconductivity, one faces there main lines of thought:[1,2] (a) new pairing mechanisms leading essentially to BCS-type superconductivity, (b) condensation of bosons (holons,[3] bipolarons,[4] etc.) preexisting above T_c (c) superconductivity due to gauge forces with excitations obeying fractional statistics.[5]

In the context of pairing theories, it has been proposed by Weinstein[6] that one-particle excitations in strong-coupling superconductors are the so-called "pairing bags."[7] A pairing bag is an excitation corresponding to a quasiparticle self-trapped in a region where the order parameter is locally depressed. This effect is realizable in small coherence length systems, where the order parameter can vary within small distances. This idea is appealing for the new superconductors where the coherence length is of the order of the distance between particles (holes in cuprate superconductors). Systems with such a short coherence length are however halfway between BCS and Bose condensation.[8] In the latter case the collective excitations involve phase modes without pair breaking.[4] In the intermediate-coupling regime it seems natural, therefore, to think of bags in which both the phase and the amplitude are modulated.

In this article we will concentrate in the strong-coupling case, with the hope that a good understanding of this limit could give us an insight about the more interesting intermediate regime. We show that bags can be built by local variations of the phase of the order parameter, in close analogy with spin polarons in the t-J model.[9–12] For intermediate particle densities the superfluid excitations strongly renormalize the one-particle spectrum.

We will be concerned with the negative-U Hubbard Hamiltonian which in the usual notation reads

$$H=-t\sum_{\substack{\langle ij\rangle\\ \sigma}} C_{i\sigma}^{\dagger}C_{j\sigma}-U\sum_i n_{i\uparrow}n_{i\downarrow}\ . \tag{1}$$

In the strong-coupling limit ($U \gg t$) the Hamiltonian in Eq. (1) can be mapped onto a Heisenberg model given by

$$H=J\sum_{\langle ij\rangle} S_i^zS_j^z-\tfrac{1}{2}(S_i^+S_j^-+S_i^-S_j^+) \tag{2}$$

with $J=4t^2/U$.

In Hamiltonian (2) the spin-up and spin-down state at site i correspond, respectively, to an empty and doubly occupied state of the fermions in (1). The longitudinal antiferromagnetic term $S_i^zS_j^z$ describes a repulsion between nearest-neighbor doubly occupied sites, while the transverse ferromagnetic term accounts for the hopping of the composite boson (electron pairs) through a virtual pair-breaking excitation. This Hamiltonian can be transformed into one involving purely antiferromagnetic interactions by means of a canonical transformation. The particle density n is related to the total magnetization through $\langle S^z\rangle=(1-n)/2$. In the spin-wave theory the ground state of Hamiltonian (2) corresponds to an ordered state of tilted spins plus zero-point fluctuations (see Fig. 1). The angle θ between the z direction and the spins is fixed by the density. This ordered phase corresponds to a superfluid phase of the composite bosons. The superfluid order parameter is given by the magnetization in the x-y plane. The orientation of $\langle S^+\rangle$ is the phase of the superfluid order parameter. In the unpolarized half-

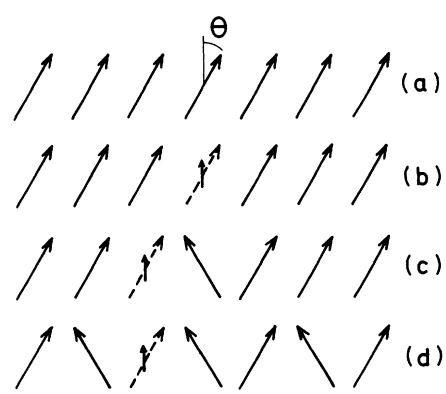

FIG. 1. (a) Classical spin image of the superfluid ground state. (b) Fermion in an otherwise undistorted superfluid background. (c) Fermion plus a superfluid distortion caused by the jump of the fermion from site i to site j. (d) Nagaoka-like state in which the fermion kinetic energy is minimized.

filled case this phase is degenerated with the density wave phase. This is clearly seen in the positive-U case through the exact mapping between the $U>0$ and $U<0$ situations discussed by Nagaoka.[13] The superfluid phase and the density wave phase map onto an antiferromagnetic ordered phase in the x-y plane and in the z axis, respectively. Clearly, in the positive-U case these two types of order differ by a rotation and are therefore degenerate.[13] In what follows we will simply use the spin language to refer to empty and doubly occupied sites. It is well known that the ground state in the mean-field approximation of Hamiltonian (2) corresponds to a BCS approximation of Hamiltonian (1). The dispersion relation Ω_q of the collective excitations ("sound waves") is linear for small q.

We consider the case of a single unpaired particle (hereafter referred to as the fermion). This case occurs if one works with an odd number of particles. The excitation spectrum of the fermion will govern the behavior of a single particle injected in the superfluid or modify the pair-breaking excitations. In the case of an unpaired particle, it is convenient to divide the Hamiltonian in two terms H_0 and H'. The first term H_0 describes the spin dynamics with the unpaired particle located at a fixed position [see Fig. 1(b)]. Zero-point fluctuations will distort the superfluid order parameter in the neighborhood of the fermion in analogy with a fixed hole in the Heisenberg model. The second term H' describes the hopping of the fermion. When the fermion jumps from site i to site j the tilted spin (which corresponds to a linear combination of vacuum and double occupation) jumps backwards from site j to site i. In this process the z component is conserved, but the phase in the x-y plane changes as shown in Fig. 1(c). This is clearly seen in the $U\to\infty$ limit if one considers a fermion added at site i of the unperturbed state. The resulting state is

$$|\phi_{i,\sigma}\rangle = C_{i\sigma}^{\dagger}\prod_{l}(u+vC_{l\uparrow}^{\dagger}C_{l\downarrow}^{\dagger})|0\rangle \ . \tag{3}$$

When the fermion jumps from site i to site j the final state corresponds to

$$|\phi'_{j,\sigma}\rangle = C_{j\sigma}^{\dagger}(u-vC_{i\uparrow}^{\dagger}C_{i\downarrow}^{\dagger})\prod_{l\neq i}(u+v_{l\uparrow}^{\dagger}C_{l\downarrow}^{\dagger})|0\rangle \ . \tag{4}$$

In this way, as the fermion moves, it distorts the superfluid background. However, the final state at site i is not orthogonal to the unperturbed one, its overlap being u^2-v^2. Consequently, the hopping matrix element can be divided into a "bare" term t_b corresponding to a jump without creating excitations and a term t' corresponding to the jump with a simultaneous creation of an excitation of the background. The bare term is simply given by $t_b=t\cos\theta$. For the half-filled band case the total magnetization is zero and $t_b=0$. Our model then reduces to the t-J model. Our first result is then the analog to the Nagaoka theorem: in the $U\to\infty(J\to 0)$ limit the ground state of the system with an unpaired particle consists of a state with a translational symmetry corresponding to $\mathbf{Q}=(\Pi,\Pi)$ (antiferromagnetic in the x-y plane), as shown in Fig. 1(d). In this structure the hopping matrix elements are $t_b=t$ and $t'=0$ and the kinetic energy of the fermion is minimized. For finite U the fermion will create a bag as a result of the competition between its kinetic energy and the energy needed to locally distort the superfluid order parameter. We estimate the radius R of the bag using an uncertainty principle calculation and obtain, in two dimensions, $R\approx[t/Jn(2-n)]^{1/4}$, where n is the superfluid density.

To put these concepts in a more quantitative way, we consider a Hamiltonian that includes the spin (superfluid) dynamics together with the distortions of the background due to the motion of the fermion. Following Ref. 11 we consider the vacuum $|0\rangle$ to be the ordered state of tilted spins. We also define hard-core boson operators a_i such that $a_i|0\rangle=0$, and

$$a_i^{\dagger}=S_i^x-i(\cos\theta S_i^y-\sin\theta S_i^z)$$

creates an excitation that corresponds to a spin flip at site i over the ordered state of tilted spins. The Hamiltonian H_t that describes the hopping of a fermion from site to site is therefore given by

$$H_t=t\sum_{\langle i,j\rangle\sigma}C_{i\sigma}^{\dagger}C_{j\sigma}\{[\sin\theta(1-a_j^{\dagger}a_j)-\cos\theta\, a_j^{\dagger}]a_i + [\cos\theta(1-a_j^{\dagger}a_j)+\sin\theta\, a_j^{\dagger}](1-a_i^{\dagger}a_i)\} \ , \tag{5}$$

where the first (second) term in square brackets describes the hopping of the fermion to a site with (without) an excitation. In terms of the boson operators, the linearized Heisenberg Hamiltonian is given by

$$H=-\frac{JzN}{4}(2\cos^2\theta+1)+Jz\sum_i a_i^{\dagger}a_i -\frac{J}{2}\sin^2\theta\sum_{\langle i,j\rangle}(a_i^{\dagger}a_j^{\dagger}+a_ia_j) -\frac{J}{2}\cos^2\theta\sum_{\langle i,j\rangle}(a_i^{\dagger}a_j+a_j^{\dagger}a_i) \ . \tag{6}$$

The complete Hamiltonian, in the spin-wave approximation, can be written as $H=H_0+H'$ with

$$H_0=\sum_{k,\sigma}E_kC_{k\sigma}^{\dagger}C_{k\sigma}+\sum_q\Omega_qb_q^{\dagger}b_q \tag{7a}$$

and

$$H'=\sum_{k,q,\sigma}M(k,q)(b_q^{\dagger}C_{k\sigma}^{\dagger}C_{k+q\sigma}+b_qC_{k+q\sigma}^{\dagger}C_{k\sigma}) \ , \tag{7b}$$

where E_k is the kinetic energy associated with the bare hopping $zt_b\gamma_k$, with $\gamma_k=1/z\sum_\delta e^{ik\delta}$, $b_q^{\dagger}$ creates a superfluid excitation with energy

$$\Omega_q^2=(zJ)^2[1+(2\cos^2\theta-1)\gamma_q^2-2\cos^2\theta\,\gamma_q] \ .$$

The matrix elements $M(k,q)$ are given by

$$M(k,q)=tz\sin\theta(\gamma_k\alpha_q+\gamma_{k+q}\beta_q) \ , \tag{8}$$

with the coherence factors $\beta_q^2=\alpha_q^2-1$ and

$$\alpha_q^2=\frac{1}{2}\left[\frac{zJ(1-\cos^2\theta\,\gamma_q)}{\Omega_q}+1\right] \ . \tag{9}$$

In the Hamiltonian (7) the distortion of the superfluid background due to the fixed fermion is neglected, and for $\cos\theta=0$ ($n=1$), our model reduces to the one considered in Ref. 11. Further refinements along the line of Ref. 14 can be easily incorporated. We evaluate the self-energy of the hole using a self-consistent diagrammatic approach in which the fermion Green's function and the self-energy are given by

$$G(k,\omega)=\frac{1}{\omega-E_k-\Sigma(k,\omega)} \tag{10a}$$

and

$$\Sigma(k,\omega)=\sum_q M(k-q,q)^2 G(k-q,\omega-\Omega_q) . \tag{10b}$$

In Hamiltonian (7) J and t are in principle independent parameters, and the present treatment can be applied for any ratio t/J. We first present results corresponding to the more interesting regime $J \ll t$, and then we briefly comment on the $J \gg t$ case.

We solved numerically the equations for the Green function (10) in a square lattice for different values of the density, and for $J=0$. In Fig. 2 we present results for $\cos\theta=0$ (the t-J model). For a 4×4 cluster our calculations of the spectral density for $\mathbf{k}=(\pi/2,\pi/2)$ are in remarkable agreement with the exact results obtained by Dagotto *et al.*[15] for that cluster size. The shape of the local density of states resembles that of the Bethe lattice with coordination number $z=4$, in agreement with the results of the self-retracing path approximation obtained by Brinkmann and Rice.[16] As expected, the fermion spectrum is incoherent in this limit. For $\cos\theta\approx0$ and $J=0$ the spectrum remains incoherent, although one could have expected the bare hopping term to create a quasiparticle pole. Results for the spectral density for different values of $\mathbf{k}$ are shown in Fig. 3.

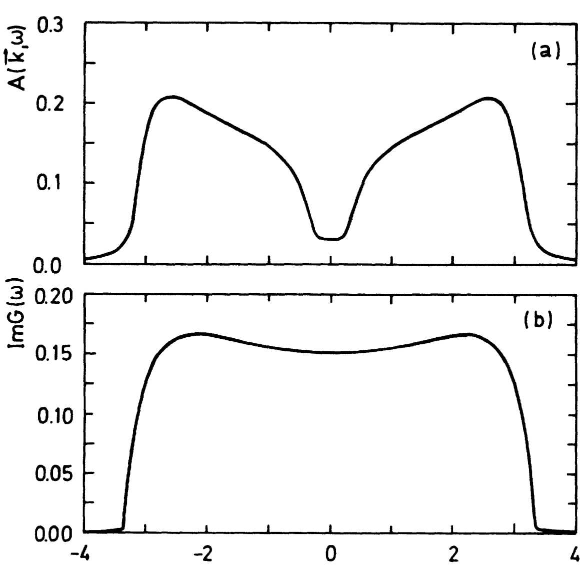

FIG. 2. (a) Spectral density $A(k,\omega)$ for a 4×4 cluster, $n=1$, $\mathbf{k}=(\pi/2,\pi/2)$, and $J=0$. (b) Local density of states for a 12×12 cluster an $n=1$.

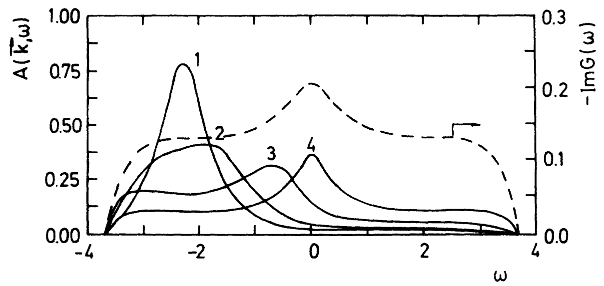

FIG. 3. Spectral density (continuous line) corresponding to the wave vector $\mathbf{k}=(0.,0.)$ (1), $\mathbf{K}=(\pi/6,\pi/6)$ (2), $\mathbf{k}=(\pi/3,\pi/3)$ (3), $\mathbf{k}=(\pi/2,\pi/2)$ (4), $n=0.5$, and $J=0$. Dashed line is the corresponding local density of states.

For $0<J\ll t$ we performed some analytical approximations to study the main features of the spectral density. In the dominant pole approximation,[12] the Green function of the hole can be written as

$$G(k,\omega)=\frac{a_k}{\omega-\omega_k}+G_{\rm inc}(k,\omega) , \tag{11}$$

where ω_k is the position of the pole and $G_{\rm inc}$ the incoherent part of G. The residue of the pole is given by

$$a_k=\frac{1}{1-\frac{\partial\Sigma}{\partial\omega}(k,\omega_k)} . \tag{12}$$

Following Ref. 12, we conclude that the spectrum in the bottom of the band is completely incoherent ($a_k=0$). It is also interesting to look for the wave vector $\mathbf{k}^*$ corresponding to the bottom of the band. For zero density ($\cos\theta=1$) the fermion moves as a free particle of wave vector $\mathbf{k}^*=0$. For the half-filled band ($\cos\theta=0$), $\mathbf{k}^*=\pi/2$. We then expect $\mathbf{k}^*$ to evolve continuously from 0 to $\pi/2$ as the superfluid density increases. Since the bottom of the band is given by the minimum of ω_k, we obtained $\mathbf{k}^*$ as the value of $\mathbf{k}$ for which

$$\nabla\omega_k=\nabla(E_k+\Sigma(k,\omega_k))=0 . \tag{13}$$

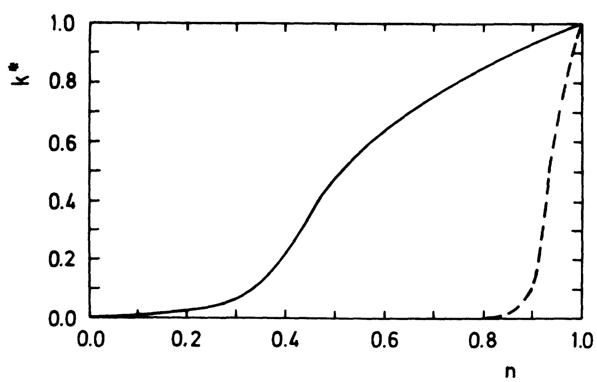

FIG. 4. Wave vector $\mathbf{k}^*$ corresponding to the minimum of the fermion dispersion relation as a function of the superfluid density for $J=0$ (continuum line) and $J=5t$ (dashed).

In the $J \ll t$ limit this expression can be simplified[12] to obtain the results shown in Fig. 4. In this approximation ($J \ll t$) $\mathbf{k}^*$ is a function of the density only. For low densities $\mathbf{k}^* \approx 0$, while for $n \gtrsim 0.5$ it increases and reaches $\pi/2$ for $n = 1$.

For $J \gg t$ Eqs. 8 can be solved using a perturbation expansion.[11] In this limit there is a quasiparticle pole carrying most of the spectral weight. This is due to the superfluid fluctuations that have a restoring effect on the distortions caused by the fermion. However, the fermion effective mass is strongly enhanced by the superfluid background. The quasiparticle pole forms a band of a width that decreases linearly with the superfluid density n. As in the previous case, the bottom of the band corresponds to a $\mathbf{k}^*$ that varies with n (see Fig. 4). In this case, $\mathbf{k}^*$ remains close to the center of the Brillouin zone for a wider range of n than for the $J \ll t$ limit.

In summary, we presented a treatment for the movement of a single particle in a superfluid background corresponding to the strong-coupling limit of the negative-U Hubbard model. The problem is analogous to that of a hole in the Heisenberg antiferromagnet in a strong magnetic field. All our results can therefore be used in the understanding of the polarized t-J model. There are, however, some differences, the collective excitations in the t-J model are magnons which carry magnetization current, while in the present model the collective excitations carry charge current. In the present treatment we study the deformations of the superfluid where the total current is zero. Our results show that for large attractive interaction it is possible to create bags where the phase of the order parameter is distorted in the surroundings of the quasiparticle, without weakening the binding energy of the pairs.

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