Superfluid Precursor Effects in a Model of Hybridized Bosons and Fermions

J. Ranninger and J. M. Robin
Centre de Recherches sur les Très Basses Températures, Laboratoire Associé à l'Université Joseph Fourier, Centre National de la Recherche Scientifique, BP 166, 38042 Grenoble Cédex 9, France

M. Eschrig
Institut für Theoretische Physik III, Universität Bayreuth, D-95440 Bayreuth, Germany
(Received 11 July 1994)

We examine how a superfluid state is approached in a system of localized bosons (tightly bound electron pairs) in contact with a reservoir of itinerant fermions (electrons). Assuming spontaneous decay and recombination between these two species, the initially localized states of the bosons change over into free-particle–like propagating states as the temperature is lowered and the superfluid transition at T_c is approached. Concomitantly a pseudogap opens up in the fermionic density of states which deepens with decreasing temperature.

PACS numbers: 67.20.+k, 05.30.−d, 74.20.−z

In order to describe the crossover [1] between weak-coupling BCS and strong-coupling bipolaronic superconductivity [2] in an electron-phonon coupled system, the boson-fermion model has been introduced [3]. It consists of a mixture of itinerant electrons (fermions) and tightly bound electron pairs (hard core bosons) of polaronic origin which can spontaneously decay into itinerant electrons and vice versa. This is a natural intuitive extension of the bipolaronic model, where the only charge carriers are tightly bound electron pairs (bipolarons) which undergo a superfluid transition below a certain critical temperature T_c. Studies of the polaron problem [4] indicate that in the intermediary electron-phonon coupling regime electrons exist in a mixture of states composed of quasilocalized bipolarons and itinerant electrons. The bipolarons then move by spontaneous decay into itinerant electrons and subsequent recombination.

The boson-fermion model has been suggested as a possible scenario for high-T_c superconductivity [5] and its thermodynamic and electromagnetic properties have been extensively studied for the superconducting state [5,6]. Assuming the bosons to be in free-particle–like itinerant states [5], the boson-fermion model shows a superconducting ground state below T_c which is approximately given by the Bose-Einstein transition condensation $k_B T_c \cong 3.3\hbar^2 n_B^{2/3}/m_B$. For typical values of the boson density ($n_B \sim 10^{22}/\mathrm{cm}^3$) and the boson mass ($m_B \sim 10$ electron masses) T_c can easily be of the order of a few hundred K, which makes this model an attractive candidate for high-T_c superconductivity.

In real materials we expect the tightly bound electron pairs (bipolarons) to be localized rather than itinerant. Nevertheless, the studies carried out on the boson-fermion model with localized bosons clearly show a superconducting ground state within mean field and random-phase approximation (RPA) [6]. It is the purpose of this Letter to investigate the normal-state properties of this boson-fermion model and in particular to show how upon approaching T_c the boson spectrum changes from a localized into an itinerant one, which is a prerequisite for superfluidity in such a system.

We define the boson-fermion model by the following Hamiltonian:

$$H = (zt - \mu)\sum_{i\sigma} c_{i\sigma}^{\dagger} c_{i\sigma} - t \sum_{\langle i \neq j \rangle \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + (\Delta_B - 2\mu) \times \sum_i b_i^{\dagger} b_i + v \sum_i (b_i^{\dagger} c_{i\downarrow} c_{i\uparrow} + \mathrm{H.c.}) . \qquad (1)$$

The localized tightly bound electron pairs are represented here by boson annihilation (creation) operators $b_i^{(\dagger)}$ with $[b_i, b_i^{\dagger}] = \delta_{ij}$, where i, j denote the sites on a lattice. We neglected any hard core effects of the tightly bound electron pairs, which is justified as long as we are in the dilute limit of the bosons. The conduction electrons are represented by fermion annihilation (creation) operators $c_{i\sigma}^{(\dagger)}$ with $\{c_{i\sigma}^{\dagger}, c_{j\sigma'}\} = \delta_{ij}\delta_{\sigma\sigma'}$. The boson and fermion operators are assumed to be commuting operators. The spontaneous decay and recombination process between bosons and fermions is described by a local interaction $v(b_i^{\dagger} c_{i\downarrow} c_{i\uparrow} + b_i c_{i\uparrow}^{\dagger} c_{i\downarrow}^{\dagger})$, where the lattice sites i represent some finite small clusters in real systems on which this exchange process is expected to take place. v denotes the strength of this interaction, and t the hopping integral for the tight binding electrons. z denotes the number of nearest neighbor sites on the lattice, and μ the chemical potential which is common to both the fermions and bosons and thus guarantees global charge conservation. The bosons having charge $2e$ are assumed to have an energy level Δ_B such that $2zt - \Delta_B$ corresponds to the energy necessary to dissociate a tightly bound electron pair (bipolaron) into two electrons on the same site.

We base our calculations of the normal state properties of this boson-fermion mixture [Eq. (1)] on the self-energy diagrams for fermions and bosons [Figs. 1(a) and 1(b)]

0031-9007/95/74(20)/4027(4)$06.00

FIG. 1. Self-energy diagrams for (a) bosons and (b) fermions.

which we determine in a fully self-consistent conserving way [7]. The expressions for the fermion self-energy $\Sigma_F(\vec{k},\omega_n)$ and boson self-energy $\Sigma_B(\vec{q},\omega_m)$ are hence given by

$$\Sigma_F(\vec{k},\omega_n) = -\frac{v^2}{N}\sum_{\vec{q}\omega_m} G_F(-\vec{k}+\vec{q},+\omega_m-\omega_n) \times G_B(\vec{q},\omega_m),$$

$$\Sigma_B(\vec{q},\omega_m) = \frac{v^2}{N}\sum_{\vec{k}\omega_n} G_F(-\vec{k}+\vec{q},-\omega_n+\omega_m) \times G_F(\vec{k},\omega_n). \quad (2)$$

$$G_F(\vec{k},\omega_n) = [i\omega_n - \epsilon_k - \Sigma_F(\vec{k},\omega_n)]^{-1},$$

$$G_B(\vec{q},\omega_m) = [i\omega_m - E_0 - \Sigma_B(\vec{q},\omega_m)]^{-1} \quad (3)$$

denote the fully self-consistent fermion and boson Green's functions, respectively. $\vec{k}$ and $\vec{q}$ denote the momenta, ω_n and ω_m are the Matsubara frequencies for fermions and bosons, respectively, and N is the number of sites.

The unperturbed fermion dispersion including the chemical potential is given by $\epsilon_{\vec{k}} = \xi_{\vec{k}} - \mu$, $\xi_{\vec{k}} = t(z - \Sigma_\delta e^{i\vec{k}\vec{\delta}})$, with δ denoting the vectors linking the nearest neighbor lattice site. The unperturbed boson energies are given by $E_0 = \Delta_B - 2\mu$, the factor 2 in front of the chemical potential taking into account that each boson is constituted of two fermions.

The boson-fermion model has been solved by perturbative methods [6] when the bosonic level lies well below the bottom of the fermionic band, i.e., $\Delta_B < 0$, and when it lies well above the chemical potential, i.e., $\Delta_B > 2\mu$. In the first case, the ground state of the system is described by a superfluid state of bosons. In the second case, the ground state is that of a BCS superconductor with bosons being only virtually excited.

The problem which interests us here is the intermediary regime where the bosonic level lies well inside the fermionic band just above the chemical potential such that for $v = 0$ the densities of both bosons as well as of fermions are finite. For that reason we choose as characteristic parameters of this model $\Delta_B = 0.4$ in units of the fermion bandwidth $D = 2zt$ and the total number of particles per site (fermions, bosons) $n = n_F + 2n_B = 1$. Δ_B is chosen to lie well inside the band, avoiding band edges or the zone center where van Hove singularities may give rise to specific effects which are not of interest in the present study. The interesting physical effects of this model are expected to occur at a temperature scale of the order of v^2, which we choose equal to 0.01 in order to cover a physically realistic temperature regime. Our choice of $\Delta_B = 0.4$ implies $n \geq n_c = 0.2952$ for $v \equiv 0$ which means that only for $n > n_c$ can Bose condensation occur if $v \to 0$. For $n < n_c$ a BCS-like superconducting state in the fermionic subsystem occurs via fermion pairs being virtually excited into the unoccupied bosonic states [6]. In the region $n \sim n_c$ the superconducting transition temperature shows a rapid rise as is first shown by an interpolation between the two limits $n < n_c$ and $n > n_c$ [6].

The self-consistent coupled equations (2) and (3) are solved by an iterative procedure in which $G_F(\vec{k},\omega_n)$ and $G_B(\vec{q},\omega_m)$ are evaluated for a set of Matsubara frequencies $\omega_n = 2\pi k_B T(\nu_n + \frac{1}{2})$ for $-100 < \nu_n < +99$ and $\omega_m = 2\pi k_B T \nu_m$ for $-100 < \nu_m < +100$. As usual we only compute the difference between the full and bare Green's functions, so that only a small number of Matsubara frequencies are necessary. We restrict ourselves in the present study to summing the k and q vectors over a one-dimensional Brillouin zone with a set of 101 equally spaced vectors for the bosons as well as the fermions. This restriction does not lead to results for the normal state which are qualitatively different from those when the sums are carried out over two- and three-dimensional Brillouin zones, as our preliminary results show. The only qualitative difference between the present study and a three-dimensional one is that in the present work we expect and indeed obtain a transition temperature equal to zero. Since we are basically interested only in how the various spectral properties of the bosons and fermions evolve as T_c is approached from above, the present analysis will provide us with a qualitative understanding of this evolution.

Convergency of the iterative solutions of the self-consistent equations (2) and (3) is obtained relatively fast for temperatures down to $T = 0.005$ in units of the fermionic bandwidth. The solutions for the fermion and boson Green's functions in terms of the Matsubara frequencies were then analytically continued to the real frequency axis and into the lower half plane using a standard Padé approximants procedure [8] in order to obtain the poles of the retarded Green's functions and hence the excitation spectra for the fermions and bosons. For bosons, the excitation spectrum is obtained by solving the equation

$$\omega - (\Delta - 2\mu) - \Sigma_B^R(q,\omega) = 0, \quad (4)$$

where $\omega = \omega_q^B - \frac{i}{2}\gamma_q^B$ and $\Sigma_B^R(q,\omega)$ denotes the retarded boson self-energy.

The real part of the boson excitations having frequency ω_q^B are shown in Fig. 2 as a function of the boson momenta qa in the entire Brillouin zone $[-\pi,\pi]$ (where a denotes the lattice constant) for different temperatures. We notice that as the temperature is decreased from $T = 0.01$ down to 0.005 the effective mass $m_B(T)$ of the

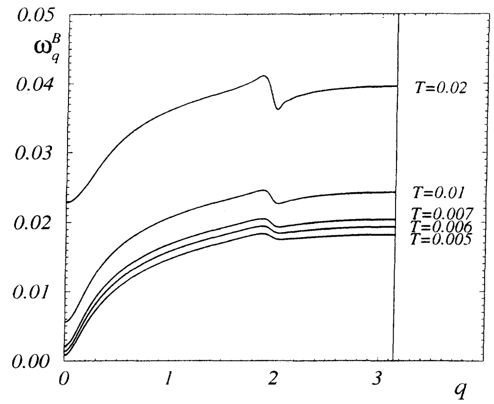

FIG. 2. Real part of the boson energies as a function of q (in units of the inverse lattice constant) and for various temperatures (in units of the fermion bandwidth). The chemical potential for bosons μ_B is set equal to zero.

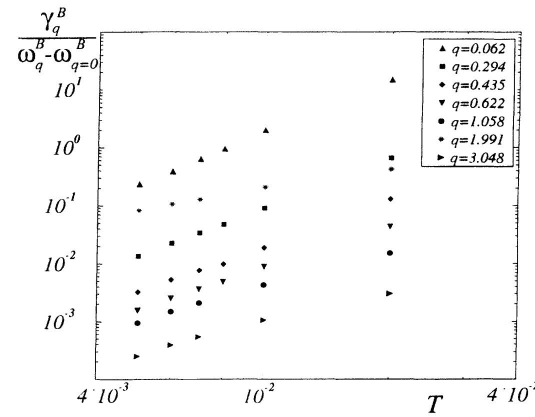

FIG. 3. Imaginary part of the boson energies as a function of temperature for various wave vectors q. The units are the same as in Fig. 2.

bosons given by $\omega^B_q = \hbar^2 q^2/2m_B(T)$ in Fig. 2, for $q \to 0$ is strongly renormalized down with decreasing temperature. We obtain $m_B(T)/m_F = 6.5$ for $T = 0.02$, 2.9 for $T = 0.01$, 2.6 for $T = 0.8$, and saturation at 2.5 as T approaches T_c ($= 0$ in our case).

The strongest renormalization of the boson spectrum occurs for small wave vectors triggered by a precursor effect of superfluidity. This behavior is indeed compatible with the behavior of $\langle b^\dagger_{\vec q} b_{\vec q}\rangle$ which tends to $n^B_{\vec q}(T)$—the Bose distribution function—and shows a strong buildup of the boson occupation for q going to zero. The overall shift of the boson spectrum shown in Fig. 2 is due to the renormalization of the chemical potential for the bosons defined by $\mu_B = -\Delta_B + 2\mu - \Sigma_B(0,0)$ which goes to zero as $T \to T_c \equiv 0$ as it should [9]. The kink in the boson spectrum occurring at $q \sim 2k_F$ (k_F denoting the Fermi vector for the unperturbed boson-fermion mixture, $v \equiv 0$) is an artifact of the one-dimensional k summations in our Eq. (3) and concerns only modes near this value. This feature is, moreover, physically irrelevant since it is only the small-q-vector boson modes which are predominantly occupied.

Evaluating the imaginary part of the poles of the boson Green's function, $-\gamma^B_{\vec q}/2$, for small $\vec q$ vectors clearly shows how upon decreasing the temperature the initially overdamped boson excitations become freely propagating modes. This is illustrated in Fig. 3 where $\gamma^B_{\vec q}(T)/[\omega^B_{\vec q}(T) - \omega^B_{q=0}(T)]$ is plotted as a function of T for a set of $\vec q$ vectors and shows a T^3 behavior except for the modes with $q \sim 2k_F$.

The onset of coherent free-particle–like motion of the bosons in the long-wavelength limit as the temperature decreases is combined with a depletion of fermionic states near the bosonic energy level, i.e., near $\Delta_B/2$. This results in fermion spectral functions which have particular three-peaked structures and which are most pronounced for k near k_F as can be seen from Fig. 4. This three peak structure comes about from a hybridization of the fermions with the bosons which is confined to a frequency regime $\omega_1 = E_0 - \Sigma_B(0,0) < \omega < \omega_2 = E_0 - \Sigma_B(0,0) + \mu$ in which $\mathrm{Im}G(k,\omega) \neq 0$. For the set of parameters in Fig. 4 we have $\omega_1 = 0.0013$ and $\omega_2 = 0.1882$ and $\mu = 0.1868$. The poles of the fermionic Green's function are given by $\omega - \epsilon_k + \mu - \mathrm{Re}G(k,\omega) = 0$. For each k vector two of the solutions lie just outside this frequency interval $[\omega_1, \omega_2]$ and thus are well-defined quasiparticle excitations. The third solution lying inside $[\omega_1, \omega_2]$ is an overdamped mode arising from strong boson-fermion exchange scattering. With increasing k the spectral weight shifts from the peak below ω_1 to that above ω_2. Because of the existence of well-defined modes for $\omega < \omega_1 < \mu$ as well as $\omega > \omega_2 > \mu$ for k near the unperturbed Fermi vector k_F, a Fermi surface in such a system cannot exist. The strongest contribution to the incoherent part (the peak inside $[\omega_1, \omega_2]$) of the spec-

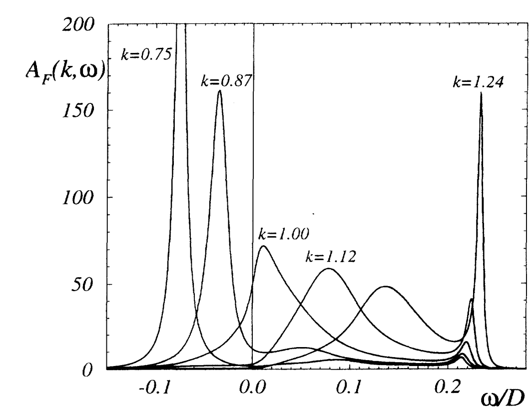

FIG. 4. Spectral function of the fermions $A_F(\vec k,\omega) = -2\,\mathrm{Im}G_F(k,\omega)$ for various k vectors near $k_F \simeq 1$ (in units of the inverse lattice constant) and for $T/D = 0.006$.

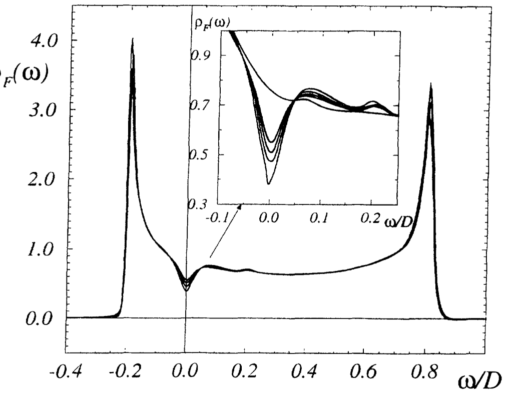

FIG. 5. The fermionic density of states for various temperatures T/D (= 0.005, 0.006, 0.007, 0.008, and 0.02) showing a deepening of the pseudogap with decreasing T.

tral function occurs in a narrow region close to $\omega = \omega_1$ due to the predominance of bosons with $q \simeq 0$. As a result this pushes away the spectral weight of the fermionic excitations, and thus leads to the formation of a pseudogap in the fermion density of states at $\omega = \omega_1$. This pseudogap deepens with decreasing temperature (Fig. 5) and eventually is expected—on the basis of previous mean field calculations [5,6] in 3D—to open up into a true gap below T_c when a global superconducting state occurs in the fermionic subsystem and ω_1 goes to zero.

The appearance of this psuedogap is not linked to the approximation in which the k summation is carried out over a one-dimensional Brillouin zone. It is a robust feature of the model, as our preliminary results of calculation show in which the k summations were carried out over two-dimensional Brillouin zones. These calculations lead to results for the spectral functions and density of states which are practically identical to those presented here. The pseudogap obtained here is a generic feature of fermionic systems with attractive interaction in the intermediary coupling regime as was recently shown for the 2D negative-U Hubbard model [10]. Already in that case it was clearly established that the pseudogap is due to the formation of some strong bosonic resonances involving tightly bound electron pairs similar to those of the bosons in the model studied here.

In the present study we have examined the qualitative features of the boson-fermion model in the normal state as T_c is approached. We showed that due to a precursor effect of the superfluid state of the bosons the latter evolve from purely localized into well-defined propagating states as the temperature is lowered. Concomitantly a pseudogap opens up in the electron density of states which deepens with decreasing temperature, expected to evolve into a true gap below T_c. The fermions near k_F are strongly correlated into pairs well above T_c, which is a general feature of fermionic systems with strong attractive interaction.

[1] A. J. Leggett, in *Modern Trends in the Theory of Condensed Matter,* edited by A. Pekalski and R. Przystawa (Springer-Verlag, Berlin, 1980); P. Nozières and S. Schmitt-Rink, J. Low Temp. Phys. **59**, 195 (1985).
[2] A. S. Alexandrov and J. Ranninger, Phys. Rev. B **23**, 1796 (1981); **24**, 1164 (1981).
[3] J. Ranninger and S. Robaszkiewicz, Physica (Amsterdam) **135B**, 468 (1985).
[4] H. B. Shore and L. M. Sander, Phys. Rev. B **7**, 4537 (1973); J. Ranninger and U. Thibblin, Phys. Rev. B **45**, 7730 (1992).
[5] R. Friedberg and T. D. Lee, Phys. Rev. B **40**, 6745 (1989); R. Friedberg, T. D. Lee, and M. C. Ren, Phys. Rev. B **42**, 4122 (1990).
[6] S. Robaszkiewicz, R. Micnas, and J. Ranninger, Phys. Rev. B **36**, 180 (1987); R. Micnas, J. Ranninger, and S. Robaszkiewicz, Rev. Mod. Phys. **62**, 113 (1990).
[7] G. Baym and L. P. Kadanoff, Phys. Rev. **124**, 287 (1961); **127**, 1391 (1962).
[8] H. J. Vidberg and J. W. Serene, J. Low Temp. Phys. **29**, 179 (1977); J. Heym, J. Low Temp. Phys. **89**, 869 (1992).
[9] N. M. Hugenholtz and D. Pines, Phys. Rev. **116**, 489 (1959).
[10] A. Moreo, D. J. Scalapino, and S. R. White, Phys. Rev. B **46**, 7544 (1992); J. J. Rodriguez-Nunez *et al.* (to be published).