Electron-hole liquid model for high-T_c superconductors: Metal-insulator transition and doping behavior

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We propose a theoretical model for high-T_c superconductivity based on the existence of two types of mobile charge carriers: electrons and hole bosons. The bosons are assumed to be mobile in CuO_2 planes and the electrons in separate parts of the crystal in order to prevent annihilation. We simulate this situation with a uniform mixture of electrons and bosons by adding a short-range repulsion between them. The model predicts the existence of a linear electronic sound mode which is analogous to the first sound in He mixtures. The electron component contributes a linear term and the sound mode a cubic term in the electronic specific heat. The transition at T_c is interpreted as a λ transition whereas the pairs are formed at a higher temperature T_{BCS}. For small hole concentrations the charge carriers form an excitonic bound state of heavy-fermion type which is immobile and hence provides an explanation for metal-insulator transition. The model predicts also the doping behavior in agreement with experiment including the pressure dependence of T_c. The specific-heat linear term is predicted to increase with pressure for hole-doped and to decrease for electron-doped superconductors. The predictions are valid for all types of high-T_c compounds and also for the new electron superconductors. The value of normalized slope of specific heat discontinuity at T_c can exceed the maximum values obtainable by the BCS and Eliashberg theories. Some features of NMR experiments can be understood.

I. INTRODUCTION

Since the discovery of high-T_c superconductors,[1] no convincing pairing mechanism has been presented to explain the phenomenon. It is therefore worthwhile to see to what extent one can progress without knowing the exact mechanism. In fact even for normal BCS superconductors a first-principle calculation of T_c or the gap parameter Δ is strictly speaking not possible. In previous papers[2,3] we proposed an electron–hole-boson liquid (EHBL) model for high-T_c superconductivity. The basic assumption of the model was the existence of both mobile electrons and mobile hole bosons[4–15] in these compounds. Since the coherence length of the paired holes is small, $\xi_0 \sim 3$–20 Å, and hence the gap Δ is very large,[16,17] it was assumed that one can treat them simply as composite bosons[18] of charge $+2e$. It was further assumed that the electrons are moving mainly in the c direction whereas the bosons are constrained to move in a-b planes.[19] We will relax this condition here so as to assume that the electrons and bosons are situated in separated parts of the crystal in order to prevent the annihilation, but the directions of their mobilities are such that the exciton bound state for small hole concentrations is localized. This would then explain the metal-insulator transition found in the high-T_c compounds. In our jellium-model calculation with uniform densities we will simulate the situation by modifying the electron-boson interaction to become repulsive at short distances to lower the annihilation rate[20] given by the radial distribution function $g_{eB}(r)$ at $r=0$. In reality the annihilation is prevented by the topology of the lattice: the bosons reside in CuO_2 planes, separated from the electrons. The stability of such a system is clearly connected with the unknown binding mechanism of the bosons. An analogous situation occurs in nuclei where the ground state may be based on a deformed Hartree-Fock but some excited states on a spherical one or vice versa. Here the system is highly anisotropic and correspondingly the problem is an order of magnitude more complicated. We want to stress that for present purposes it is not necessary to fix the internal structure of the bosons to be a hole pair. All we need here is their charge and the fact that they decay into two holes at temperatures higher than T_c. Therefore within the present approach the scenarios which posess the same boson-fermion structure are equally possible. However, we want to use in our presentation, as long as possible, concepts from BCS, such as pairs, pair breaking, etc., without actually implementing the BCS as the sole binding mechanism of the bosons. Similarly the "electrons" here can be taken to be more exotic fermions, but with the correct charge $Q=-e$.

Our model then essentially consists of a mixture of electrons and hole bosons in analogy with the electron-hole liquid in semiconductors.[20,21] The evidence for the existence of both types of carriers in these compounds is born out by the Hall measurements[19] and there is some evidence[17,22] for the existence of pairs well above T_c. The main evidence of mobile electrons comes from low-temperature specific-heat experiments.[23–26] It has

become increasingly clear that the linear term in the specific heat is not due to the impurities but is most likely an intrinsic property of high-T_c superconductors. Although some controversy remains,[27] we shall nevertheless assume the existence of mobile electrons also below T_c.

The behavior of the resistivity in the magnetic field for $T_c \leq T \leq T_0$ seems to indicate a two-dimensional (2D) behavior[28,29] near the Kosterlitz-Thouless temperature T_c. This merely means that the 2D-plane structure becomes dominating in the fluctuations but does not in any way invalidate the present 3D model. The behavior of many other quantities such as specific heat can also be very complicated in this temperature range.[30] Since according to the present model at T_c essentially an ordinary λ transition occurs, we will define yet another temperature $T_{\rm BCS} > T_c$ to be the point where all hole pairs are broken. If the mobile hole pairs exist for $T > T_c$ they also can cause unusual experimental effects together with the mobile electrons which we assume to exist even below T_c. The size of the discontinuity in the specific heat at T_c depends exponentially upon the temperature difference $T_{\rm BCS} - T_c$ and hence can show wide variation,[30,31] as is also observed experimentally. The temperature $T_{\rm BCS}$ can be sensitive to the impurities. Needless to say the impurities can cause variation of the density and effective mass of the mobile electrons and thereby cause sample dependence in quantities like the specific-heat linear term. The impurities can cause part of the mobile electrons to go from extended states to localized states.

The framework of our model is qualitatively presented in Fig. 1. Above $T_{\rm BCS}$ one has normal metal. When $T_c < T < T_{\rm BCS}$ the conduction is partly due to the pairs but the superfluid density $n_s=0$. In this temperature range we may call the system a BCS metal. Below T_c, one has $n_s > 0$ and the system is superfluid and superconducting. There is ample experimental evidence showing abnormal behavior of resistivity above T_c. Some of the latest ultrasound measurements[32] combined with specific-heat measurements in $Bi_2Sr_2CaCu_2O_8$ at T=240 K show a second-order transition where the ultrasound attenuation shows very similar behavior as the one observed in normal BCS superconductors. Therefore this temperature could be interpreted as the point where bosons are formed.[22] One should at least keep this possibility open although the normal explanation would be a structural transition.[32] An abrupt drop in the ultrasound attenuation can be a sign of pair formation like it is in the case of normal superconductors. This picture is further clarified by recent electron-energy-loss experiments[17] on single crystals of $YBa_2Cu_3O_7$ and $Bi_2Sr_2CaCu_2O_8$ (2:2:1:2). The gap seems to exist well above T_c and the size is $2\Delta = 7.8k_BT_c$ as compared with $\Delta = 1.76k_BT_{\rm BCS}$ for the normal superconductors. The two conditions together give $T_{\rm BCS} = 2.2T_c$ which for the 2:2:1:2 compound lies at about 200 K. Clearly then the present approach can be looked upon as being a generalization of BCS theory.

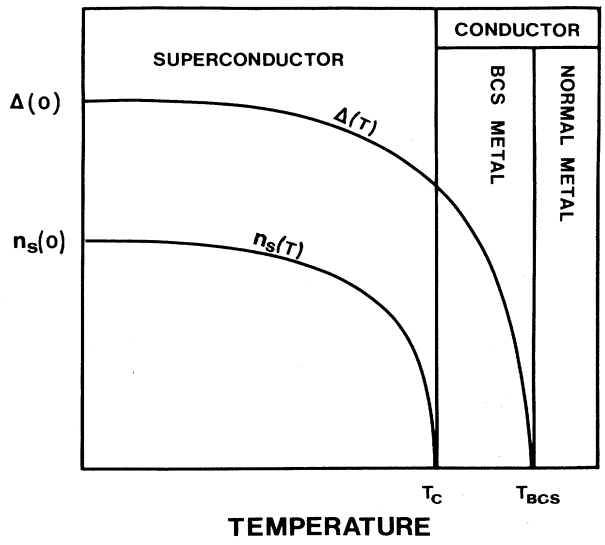

FIG. 1. Qualitative picture used as a working hypothesis: The superfluid density $n_s(T) \neq 0$, below T_c, and the gap $\Delta(T) \neq 0$, below $T_{\rm BCS}$.

It was pointed out in Ref. 2 that a mixture of electrons and bosons exhibits a low-lying acoustic phonon branch and a high-lying plasmon branch at T=0. The optical plasmon together with the pair breaking effect will be neglected here since they both lie higher in energy. The electron-phonon spectrum deviates from linearity before the mode gets dissolved into the particle-hole continuum at some high value of k. This happens at an energy much higher than the gap.

Since the pairs in high-T_c superconductors are assumed to be in $^1S_0$ state the order parameter is formally the same as in the BCS theory or in the superfluid mixture of ^{3}He and ^{4}He. In the latter system several sound modes exist. The analogous modes most likely also exist here. In the present work we will explore the consequences of the electron sound mode which corresponds to the first sound in the He mixtures. At present we still have no direct experimental evidence of the electron sound mode.

We should stress that within the present model the bosons and fermions have opposite charges as compared with the model proposed by Friedberg and Lee.[33] This makes it possible to understand the metal-insulator transition as the exciton bound-state formation for low hole concentrations. In this case also the crucial sound mode would be completely Landau damped. By exchange of the roles of electrons and holes one can understand the electron superconductors[34] as well. It was shown by Schafroth 35 years ago that ideal charged boson gas is a superconductor for all densities. The validity of the Schafroth solution has been recently questioned by Friedberg, Lee, and Ren.[35] This criticism does not concern our approach because we also have the electron component present which makes the screened boson-boson interaction short ranged, and furthermore we go beyond the ideal-gas approximation.

The plan of the paper is as follows: In Sec. II we present the mathematics of the electron–hole-boson liquid model together with some numerical results at $T=0$. We present evidence that Landau damping determines the end points in hole concentration where T_c becomes zero. In Sec. III we discuss the role of the electron sound mode in determining T_c as a function of electron and boson densities. We also derive an approximate analytical expression for the behavior of T_c in doping. The pressure dependence of T_c, including the asymmetry effect[36] found in hole-doped[37] and electron-doped[38] superconductors, is discussed in Sec. IV. In Sec. V we discuss the specific heat at low temperature and the specific-heat jump at T_c in the light of He liquids, including also the pressure dependence of the linear and cubic terms.

II. ELECTRON–BOSON-HOLE LIQUID

The starting point of our model is the coexistence of mobile electrons of density n_e and mobile hole bosons with density n_B on the lattice. The effective masses are m_e^* and m_B^*. At first we include only the Coulomb interactions between the component particles. The interaction between electrons and bosons is attractive. We cannot perform the full scale calculation on a lattice but will have to approximate the lattice with a neutralizing background which supports the mixture of electrons and bosons of uniform densities. We believe that this model is accurate in the long-wavelength limit which is sufficient for calculation of the elementary excitations and then the superfluidity. It turns out that for long wavelengths and high density one can work out the consequences of the model in closed form. This means that we can calculate T_c as a function of n_e and n_B analytically. Hence we also get a formula for T_c in doping. The electrons and bosons may screen each other completely or partially. If $n_e = 2n_B$ one has local charge neutrality, otherwise nonmobile background charges keep the system neutral. Although we cannot carry a full-scale calculation on the lattice, the existence of the lattice is ultimately crucial to our model because only then do we have the situation where the electrons and holes never meet in space and get annihilated, as they do in the case of normal electron-hole liquid in semiconductors.[20] We will simulate the existence of the lattice by introduction of a short-range repulsion in the v_{eB} channel. This makes $g_{eB}(0)$ small and hence annihilation also small.

The Hamiltonian for the mixture system is

$$H = -\frac{\hbar^2}{2m_e^*}\sum_{i=1}^{N_e}\nabla_i^2 - \frac{\hbar^2}{2m_B^*}\sum_{i=1}^{N_B}\nabla_i^2 + \sum_{1\le i<j\le N_e} v_{ee}(r_{ij}) + \sum_{1\le i<j\le N_B} v_{BB}(r_{ij}) + \sum_{1\le i\le N_e}\sum_{1\le j\le N_B} v_{eB}(r_{ij}) \,. \tag{1}$$

Even in the case of a simple jellium calculation, approximations such as random phase are not accurate enough for the radial distribution functions. We therefore resort to Jastrow ansatz for the ground-state wave function

$$\psi = \prod f_{ee}\prod f_{BB}\prod f_{eB}\Phi_e\Phi_B, \tag{2}$$

where $f_{\alpha\beta}$ are the two-body correlation factors, Φ_e is the Slater determinant of plane waves for electrons, and $\Phi_B=1$. Clearly at this stage we ignore all effects coming from the intrinsic structure of the hole pairs in Φ_B. Although we will most of the time use approximate analytical expressions it is important to also have a more accurate numerical scheme at one's disposal. The expectation value of the Hamiltonian can be expressed in terms of the radial distribution functions $g_{ee}(r)$, $g_{eB}(r)$, and $g_{BB}(r)$ alone if one makes use of the hypernetted chain connections[39]

$$g_{\alpha\beta}(r) = f_{\alpha\beta}^2(r)e^{N_{\alpha\beta}(r)+E_{\alpha\beta}(r)} \,, \tag{3}$$

where $N_{\alpha\beta}$ is the nodal function and $E_{\alpha\beta}$ the bridge function which is small for Coulomb liquids and will be neglected here. Minimization of energy then enables one to write Euler-Lagrange (EL) equations in terms of the radial distribution functions $g_{\alpha\beta}(r)$ alone in the form

$$-\frac{\hbar^2}{2m_{\alpha\beta}}\nabla^2\sqrt{g_{\alpha\beta}} + [v_{\alpha\beta}(r) + w_{\alpha\beta}(r)]\sqrt{g_{\alpha\beta}} = 0 \,, \tag{4}$$

where

$$\frac{1}{m_{\alpha\beta}} = \frac{1}{m_\alpha} + \frac{1}{m_\beta} \,.$$

The 2×2 matrix of induced potentials is given by[39]

$$w(k) = -\frac{\hbar^2k^2}{4}\,[M^{-1}S + SM^{-1} - 2M^{-1} + (SMS)^{-1} - (S_FMS_F)^{-1}] \,, \tag{5}$$

where

$$S_F = \begin{cases} \frac{3}{4}\frac{k}{k_F} - \frac{1}{16}(\frac{k}{k_F})^3, & k < 2k_F \\ 1, & k \ge 2k_F, \end{cases} \tag{6}$$

$$S = \begin{pmatrix} S_{ee} & S_{eB} \\ S_{eB} & S_{BB} \end{pmatrix} \,, \quad M = \begin{pmatrix} m_e^* & 0 \\ 0 & m_B^* \end{pmatrix} \,. \tag{7}$$

The liquid structure factors $S_{\alpha\beta}(k)$ are the Fourier transforms of the corresponding radial distribution functions $g_{\alpha\beta}(r)$ multiplied by $\sqrt{n_\alpha n_\beta}$. The main interactions $v_{\alpha\beta}(r)$ are Coulombic except at short distances where one may try to simulate the effect of the lattice by adding a repulsive part in v_{eB}. One can transform the EL equations into k space and prove that all $S_{\alpha\beta}(k)$ behave linearly at small k in the case of Coulomb forces and also with the added repulsion.

Once the structure factors $S_{\alpha\beta}(k)$ are known, the collective excitations for the mixture are obtained by diagonalization of the matrix

$$0.5\hbar^2k^2S^{-1}M^{-1} \ . \tag{8}$$

The spectrum turns out to have a plasma branch and a phonon branch with linear dispersion $\varepsilon \sim \hbar u_e k$ which one obtains without actually solving the Euler-Lagrange equation.[2] In a real lattice calculation the linearity would remain but the associated sound velocity would show directional dependence similar to the accoustic modes including the Brillouin zone structure. This has been demonstrated by a recent superlattice calculation[40] where electrons and bosons reside on separate, parallel layers repeating ad infinitum. This 3D-layer structure coupled with Coulomb forces develops a nonisotropic sound mode with velocity exceeding the 2D Fermi velocity. Since such calculations are an order of magnitude more difficult, the aim here is to show that the present uniform 3D model already contains the essential physics. Using purely Coulomb potentials for $v_{\alpha\beta}$, exploratory calculations were done in Ref. 3 by varying the masses and densities in order to show that the model possesses properties needed for high-T_c superconductors. We define the number densities n_e, n_B and concentrations $x_B = x$ and $x_e = 1 - x$ such that

$$n_B = xn_0 \ , \quad n_e = (1-x)n_0 \ , \tag{9}$$

where n_0 is the total density and r_0 is given by $n_0 = 0.75/\pi(r_0a_0)^3$, $a_0 = \hbar^2/m_ee^2$. The local charge neutrality corresponds to boson concentration $x = \frac{1}{3}$.

The Euler-Lagrange equations are highly nonlinear and hence difficult to solve. Ultimately one needs to solve them to obtain good accuracy for quantities like electron sound velocity u_e at realistic densities. They were solved in Ref. 3 by an iteration procedure in k space which is a generalization of the method used in Ref. 41 for a single-component case. Since the effective masses and the component densities are still largely unknown in high-T_c materials, their search would require a large amount of numerical work unless approximate analytical solutions can be found for guidance. Fortunately such an approximation exists for large total density n_0 and long wavelengths: the generalization of the uniform limit approximation to multicomponent systems. In connection with metallic hydrogen this has been discussed in Ref. 42. In the single-component case one obtains for the Fourier transform of the pseudopotential $u(r) = 2\ln f(r)$ the uniform limit approximation by

$$nu(k) = \frac{1}{S_F} - \frac{1}{S} \ ,$$

where n is the density and $S_F(k)$ is the structure factor from Eq. (6) for the uncorrelated electron gas and $S(k)$ contains the effect of correlations. Here we have to generalize the definitions of Ref. 42 to allow arbitrary electron and boson densities, the Bose statistics, and the charge $2e$ for the second component. We define new 2×2 matrices for the liquid structure factors $\hat{S}(k)$, potentials $\hat{V}(k)$, and pseudopotentials $\hat{u}(k)$ in the following way:

$$\hat{S}_{\alpha\beta}(k) = S_{\alpha\beta}(k)\sqrt{m_\alpha m_\beta} \ , \tag{10}$$

$$\hat{V}_{\alpha\beta} = v_{\alpha\beta}(k)\sqrt{(n_\alpha n_\beta)/(m_\alpha m_\beta)} \ , \tag{11}$$

$$\hat{u}_{\alpha\beta} = u_{\alpha\beta}(k)\sqrt{(n_\alpha n_\beta)/(m_\alpha m_\beta)} \ . \tag{12}$$

Similarly we define matrix $\hat{\varepsilon}_F$ to be

$$\hat{\varepsilon}_F(k) = \frac{2\hbar^2k_Fk}{3m_e^*}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \ . \tag{13}$$

The long-wavelength limit of the collective excitations are now determined according to Eq. (8) by diagonalization of the matrix

$$\varepsilon^2(k) = (\tfrac{1}{2}\hbar^2k^2\hat{S}^{-1})^2 = \hat{\varepsilon}_F(k)^2 + \hbar^2k^2\hat{V}(k) \ . \tag{14}$$

For purely Coulombic interactions the high-density limit of the electron sound velocity for the linear mode is given by

$$u_e = \frac{\hbar k_F}{m_e^*}\Gamma_c = v_F\Gamma_c \ , \quad \Gamma_c = \frac{2}{3}\sqrt{\frac{1}{1+\omega_e^2/\omega_B^2}} \ , \tag{15}$$

where the electron and boson plasma frequencies are defined by

$$\omega_e^2 = 4\pi e^2n_e/m_e^* \ , \quad \omega_B^2 = 16\pi e^2n_B/m_B^* \ . \tag{16}$$

The plasma frequency of the mixture is given by $\omega_p = \sqrt{\omega_e^2+\omega_B^2}$.

It is seen from Eq. (15) that $\Gamma_c < 1$ for all concentrations and mass ratios. This means that the sound mode lies inside the particle-hole continuum since $u_e < v_F$. The mode may therefore be Landau damped. Otherwise the general behavior $u_e(x)$ is of correct form to explain the behavior of T_c as a function of the hole concentration, as was explained in Refs. 2 and 3. It was mentioned earlier that in order to prevent the electrons and bosons from annihilating each other one should add a repulsive force at short distances. Such a force can simulate the effect of the lattice where the electrons and holes can in reality be confined to different planes. Surprisingly such a force, when added to the potential matrix $\hat{V}(k)$, would also increase the velocity u_e by an additional factor:

$$\begin{aligned} u_e &= v_F\Gamma(x) \ , \\ \Gamma(x) &= \Gamma_c(x)\sqrt{1+ck_Fm_e^*} \ , \end{aligned} \tag{17}$$

where $c = 3V_oa^3/\hbar^2\pi$ is a positive constant determined by the repulsive potential (here we choose Yukawa potential $aV_oe^{-r/a}/r$). The plasma frequency ω_p is independent of the repulsion. The situation is shown in Fig. 2, which is obtained by numerical solution of the Euler-Lagrange equations with the parameters $m_e^* = m_e, m_B^* = 0.5m_e, V_0 = 1$ Ry, $a = 2a_0$, and $r_0 = 1.5$.

It is seen that near the end points x=0 and 1 there exist points x_1 and x_2 such that $u_e(x_1) = v_F(x_1)$ and $u_e(x_2) = v_F(x_2)$, but with $x_1 < x < x_2$ one has $u_e(x) > v_F(x)$. Hence in this region $u_e(x)$ behaves like

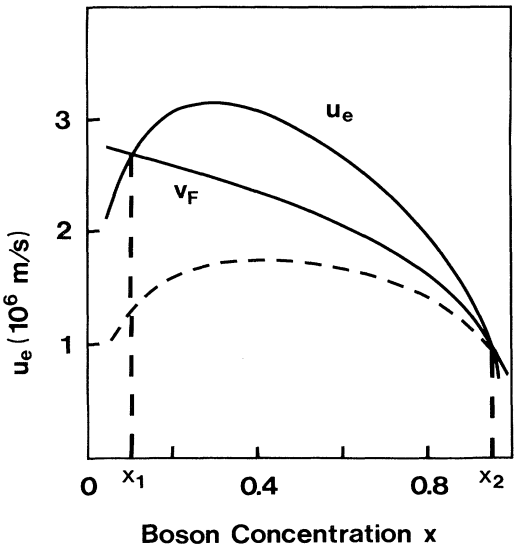

FIG. 2. The velocity of sound u_e as a function of boson concentration x: the solid line with repulsion included, the dashed line with pure Coulomb force. The Landau points x_1 and x_2 are determined by the crossing points of u_e and v_F.

zero sound mode does in ^{3}He with respect to the particle-hole continuum. Since also $v_F(x)$ vanishes at $x = 1$ the point x_2 is very close to 1, whereas x_1 can be some distance away from x=0. This circumstance in fact is exactly what is needed to explain the metal-insulator transition and the experimental behavior found in essentially all the high-T_c compounds under doping. The regions

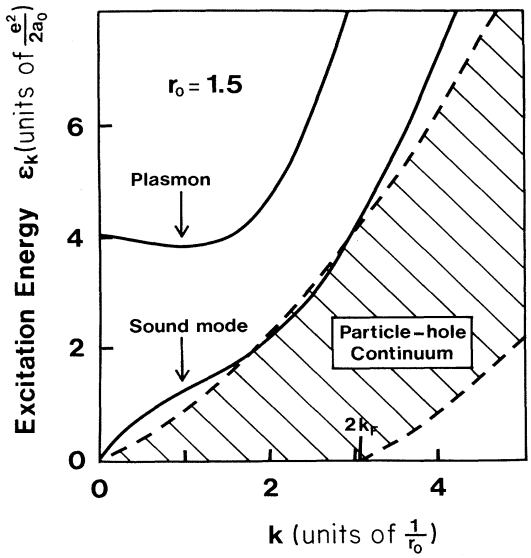

FIG. 3. The excitation spectrum of the EHBL model with the condition of local charge neutrality at the total density r_0=1.5.

around the Landau points x_1 and x_2 require a more thorough study than is possible here, to determine the exact behavior of u_e.

Before closing the discussion of the model it should be mentioned that the excited-state wave function can be written in the Feynman form

$$\psi_k = \left(A(k) \sum_{i=1}^{N_e} e^{i\mathbf{k}\cdot\mathbf{r}_{ei}} + B(k) \sum_{i=1}^{N_B} e^{i\mathbf{k}\cdot\mathbf{r}_{Bi}} \right) \psi_0 \ , \qquad (18)$$

where A and B are determined by the secular equations (14). Here ψ_0 is the exact ground-state wave function. The wave function of Eq. (18) can be utilized to evaluate various matrix elements connected with the linear mode in the gap. This wave function is known to be exact for small k. The excitation energy is shown in Fig. 3 with the same parameters as in Fig. 2.

III. T_c AS λ TRANSITION: DOPING

Since the low-energy excitations by which the bosons are depleted from the condensate are longitudinal sound waves, the situation here is similar to He liquids,[43] in particular the mixture of ^{3}He and ^{4}He. The particle-hole excitations will not deplete the Bose condensate, but will contribute to the linear term in the specific heat. The above theory was done at T=0. The properties of the system at finite temperatures are in principle obtained from the spectrum of elementary excitations in analogy with the He mixtures. Via the two-fluid model the superfluidity is related to the phonon-roton spectrum. In Fig. 4 we illustrate the situation by comparing our spectrum with the phonon-roton spectrum of a He mixture. Clearly the electron sound mode is analogous to the phonons in the He mixture. The maxon-roton part corresponds to the pair-breaking excitation shown with an isotropic gap.

According to the two-fluid model the boson component remains superfluid as long as the density of sound mode excitations is less than n_B, the density of bosons. At T_c they become equal. If that condition is solved for T_c one obtains the basic doping formula

$$k_B T_c = \left(\frac{45}{2\pi^2} \frac{m_B^* n_B}{\hbar^2} \right)^{1/4} (\hbar u_e)^{5/4} \ , \qquad (19)$$

which gives T_c as a function of the component densities. The pair-breaking excitations would modify this formula, but for simplicity we ignore them here because $k_B T_c \ll 2\Delta$ and Δ is largely unknown. The electrons, in analogy with He mixtures,[44] are assumed to be part of the normal liquid. The exact Landau condition for the normal part of the liquid would be at T_c,[45]

$$\rho_e(T_c) + \rho_B(T_c) = m_B^* n_B + m_e^* n_e \ ,$$

where ρ_e and ρ_B are the mass densities of electron and boson excitations defined by the Fermi and Bose distribution functions. Due to the wave function (18) the density $\rho_e(T_c)$ is affected by the sound mode excitations and the

normal particle-hole excitations. The density $\rho_B(T_c)$ is determined by the sound mode excitations and the quasiparticle excitations. At this stage the electron excitation mass density $\rho_e(T)$ can be eliminated by the charge conservation discussed in connection with the pressure dependence below. This gives $\rho_B(T_c) = m^* n_B$, which leads to Eq. (19). Hence the boson component goes superfluid as if the electron component did not exist if the charge conservation is used. However, the electron sound velocity depends upon the electron density and effective mass. It turns out that the fitting of the pressure dependence (see Fig. 6) requires that the electrons are light and the bosons heavy. At the charge neutrality point $n_e = 2n_B$, the electrons screen the heavier bosons completely. Hence the screened interaction between bosons is short ranged and the existence of the sound mode becomes understandable on the basis of liquid ^{4}He alone without any detailed calculations. For other density ratios the excess charge is screened by the background and the detailed theory presented in the previous chapter is needed. It turns out that we will obtain satisfactory understanding of doping, specific heat, and the pressure dependence with this simple formula.

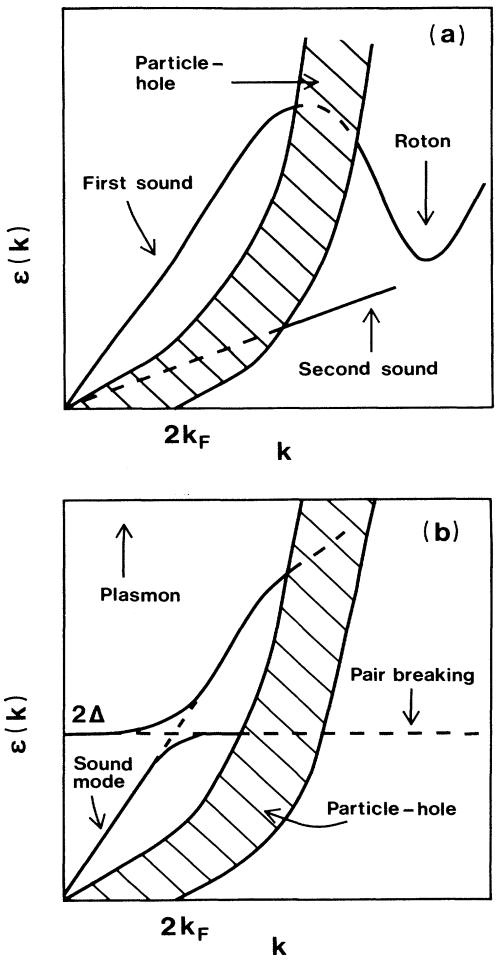

FIG. 4. (a) The phonon, maxon, roton spectrum of a mixture of ^{3}He-^{4}He. (b) The corresponding spectrum for the EHBL model. Except for the pair breaking they are very similar. The crossing of the electron sound mode and the pair breaking is shown with an isotropic gap 2Δ. If the gap was a diminishing function of k, the lower branch would look very much like the phonon-roton spectrum of the He mixture.

From here on the EHBL model is analogous with a mixture of ^{3}He and ^{4}He, where it is known that T_λ of ^{4}He comes down when the ^{3}He concentration is increased. Similarly here when electron concentration is decreased, which means increasing the boson concentration x, T_c goes up, until it again comes down following the behavior of u_e, shown in Fig. 2. The minimum boson concentration is determined by the Landau damping point x_1, as was discussed in Sec. II. Below this boson concentration the excitonic bound state of electrons and bosons may occur in analogy with the electron-hole liquid.[21] According to the assumptions, these "heavy fermions" are localized. Hence for $x < x_1$ we have an insulator. Taking over the results for u_e from Eq. (17) in Sec. II, we obtain the doping formula

$$k_B T_c = \left(\frac{45}{2\pi^2}\frac{m_B^* n_B}{\hbar^2}\right)^{1/4}\left(\frac{\hbar^2 k_F}{m_e^*}\right)^{5/4}[\Gamma(x)]^{5/4} . \tag{20}$$

Since most of the parameters are still largely unknown we have reduced Eq. (20) to the following approximate but simpler form:

$$T_c(x) = A(x_2 - x)^{5/12}(x - x_1)^{5/8}x^{1/4} . \tag{21}$$

The exact behavior of u_e and hence T_c near Landau points requires further study. In writing down this doping formula we have assumed that while the hole concentration is increased, the concentration of mobile electrons goes down but the total density n_0 of Eq. (9) stays roughly constant. Also the effective masses are assumed to remain constant during the doping. Although it is not self-evident, we have further assumed that at the Landau-damping points x_1 and x_2 the u_e vanishes and hence also T_c=0. The main argument for the vanishing of u_e at x_1 and x_2 is as follows: When u_e gets small the sound mode goes through the particle-hole continuum. At the right edge of the continuum the sound mode is pushed down by the particle-hole states above and the perturbed mode may have zero energy at finite k, which is a signal for an instability.

The results for La-based,[46–49] Y-based,[50] and Tl-based[51] superconductors are shown in Figs. 5. A search was done for parameters A and x_2. The point x_1 was obtained by simple proportionality between the hole concentration scale and the boson concentration x. It is seen that the formula (21) gives a good qualitative account of the experimental results. It is somewhat unclear how we should connect our theoretical scale x to the doping variables in these compounds. There seems to be some controversy also in the experimental values of hole

concentrations obtained with different methods.[15] If the bosons also act as mobile charge carriers for $T > T_c$ the Hall experiments need to be reexamined. Clearly the vast amount of data can be utilized, in combination with the specific-heat data, to fix the values of the parameters such as effective masses and the strength of the repulsive force needed to fit the Landau damping points.

Due to the deviations from linearity of the electron sound mode at the crossing point in Fig. 4, some corrections to Eq. (19) are expected at such high temperatures, but at least the qualitative features will remain.

It is well known[44] from He mixtures that the fermion component moves with the normal component of the liquid, therefore here also the supercurrent is determined by the superfluid velocity in the form $\mathbf{J} = (2e\hbar/m_B^*)\nabla\Phi$, where the order parameter is $\Psi = \sqrt{n_s}e^{i\Phi}$. The proof of the Meissner effect for $T < T_c$ should follow along the lines of discussion in the BCS case.[52,53] To obtain anything meaningful for critical currents one must wait for the present theory to be formulated on the lattice.[4,40]

IV. PRESSURE ASYMMETRY IN ELECTRON-DOPED AND HOLE-DOPED SUPERCONDUCTORS

One can now easily derive an approximate formula also for the pressure dependence of T_c. We regard it first as a function of component densities $T_c(n_e, n_B)$ and then

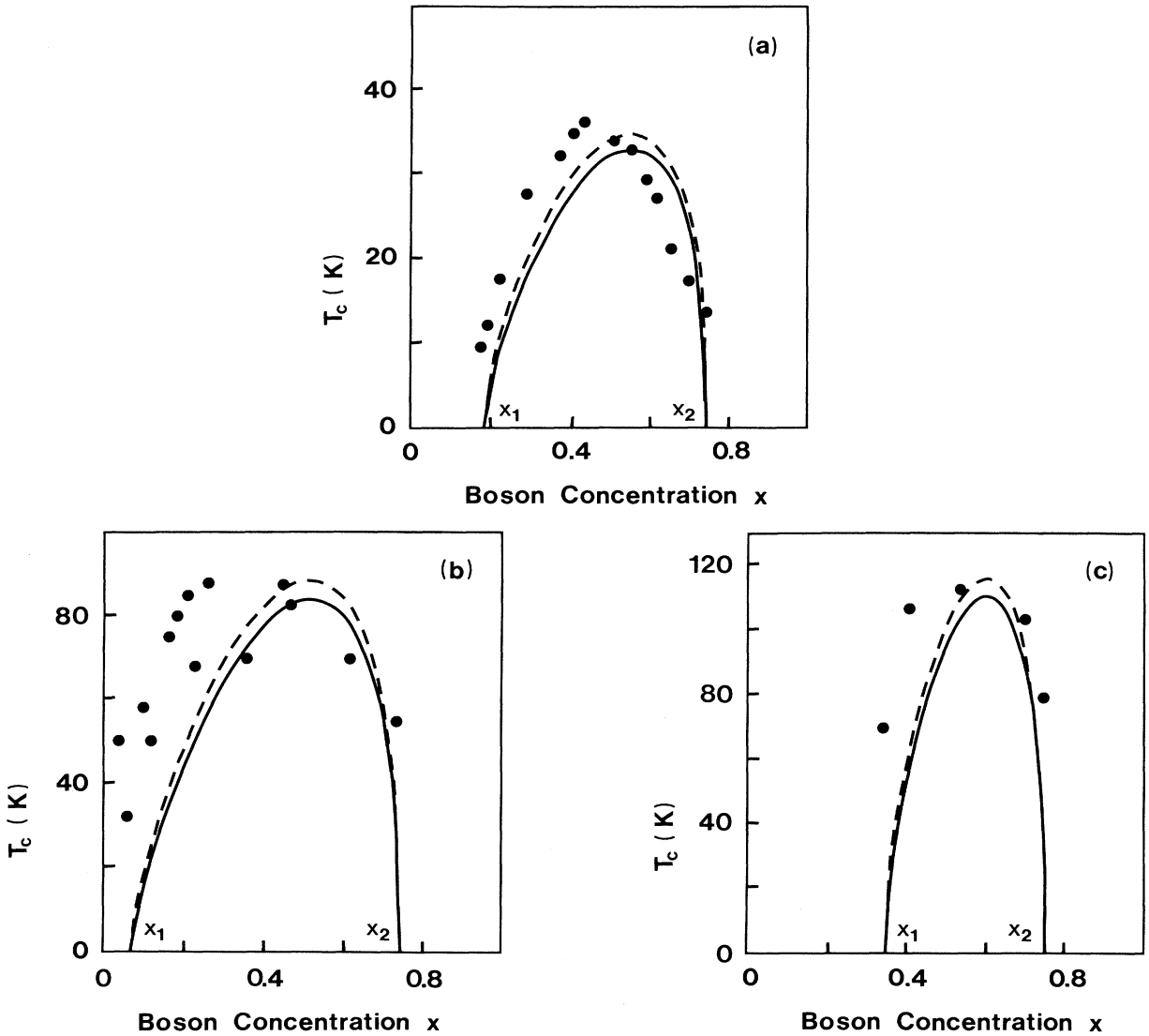

FIG. 5. Transition temperature T_c vs the boson concentration x. The experimental data in our scale are compared with the results of the present calculation. The dashed line shows the result with the repulsion included by multiplying Eq. (21) by $[1 + c'(x_2 - x)^{1/3}]^{5/8}$ with c'=0.1. (a) $La_{2-x}Sr_xCuO_4$: A=140, x_2=0.75, and Refs. 46–49; (b) Y-based compounds: A=300, x_2=0.75, and Ref. 50; (c) Tl-based compounds: A=650, x_2=0.75, and Ref. 51.

require the conservation of charge in the form $2n_B - n_e = \bar{n}$ =const. In fact $\bar{n}$ should be the carrier density one measures in a Hall experiment if both electrons and bosons are the mobile charge carriers for $T > T_c$, as our model presupposes. This statement makes sense only if the directions of mobilities are restricted.

To obtain the pressure dependence it is convenient to calculate the constrained logarithmic derivative:

$$D = \frac{1}{T_c}\frac{dT_c}{dP} = \left(\frac{\partial \ln T_c}{\partial n_B}\frac{\partial n_B}{\partial P} + \frac{\partial \ln T_c}{\partial n_e}\frac{\partial n_e}{\partial P}\right)_{\bar{n}} = \kappa_e n_e \left(\frac{1}{2}\frac{\partial \ln T_c}{\partial n_B} + \frac{\partial \ln T_c}{\partial n_e}\right)_{\bar{n}} , \quad (22)$$

where $\kappa_e = (r_0 m_e^*/6.13 x_e^{1/3})^5$ GPa^{-1} is the compressibility of the electron gas.

By Eqs. (17) and (19), the derivative D would simply be given in terms of the compressibility of the electron gas and the concentrations by

$$D = \left(\frac{5}{12} + \frac{7}{16\mu} - \frac{5}{8}\frac{2+\mu}{4\mu + M} + \frac{5}{24}\frac{c'(1-x)^{1/3}}{1 + c'(1-x)^{1/3}}\right)\kappa_e , \quad (23)$$

where $M = m_B^*/m_e^*$, $\mu = n_B/n_e$, and $c' = c\sqrt[3]{2.25\pi} m_e^*/r_0$.

The exact relation between the compressibilities κ_e, κ_B, and $\bar{\kappa}$ would be

$$n_e\kappa_e - 2n_B\kappa_B = \bar{n}\bar{\kappa} . \quad (24)$$

At the local charge neutrality point $\bar{n} = 0$ and hence κ_B can be eliminated by $n_e\kappa_e = 2n_B\kappa_B$. We continue to use this approximation also for other nearby concentrations because calculation of $\bar{\kappa}$ could bring in the whole complexity of the crystal.

From Eq. (23) one observes that function D becomes infinite for the boson concentration x=0 and 1:

$$\lim_{n_e \to 0} D \sim 5\kappa_e/12 , \quad \lim_{n_B \to 0} D \sim 7n_e\kappa_e/16n_B . \quad (25)$$

The singularities at both ends are cut away by the Landau points x_1 and x_2 discussed in Sec. II. The qualitative behavior is similar to the one observed recently[54] for $La_{2-x}Sr_xCuO_4$. In particular the gradient stays positive irrespective of x. A tentative comparison with experiment[54] is given in Fig. 6. We have used the compressibility of electron gas with r_0=3.65. The use of crystal compressibility would give an order of magnitude smaller D.

The electron-doped superconductors obey the same formalism with roles of electrons and holes being interchanged. In the formulas (22)–(25) m_B is the mass of an electron pair and m_e, κ_e become m_h, κ_h of the mobile holes. Since the energy density for the holes is negative the compressibility κ_h will be negative. Therefore T_c will diminish with pressure for electron-doped superconductors. This agrees with the experiment as is shown in Fig. 6. A more detailed discussion of the asymmetry effect is given in Ref. 36.

If we did the calculation with positive charge for the fermions, most of the formulas in the preceding sections would remain, provided that we add an extra attractive force between the boson and fermion. This would prevent the Landau damping of the sound mode. However, the pressure can no longer be calculated by Eqs. (22) and (23). In fact the most probable outcome is that the co-

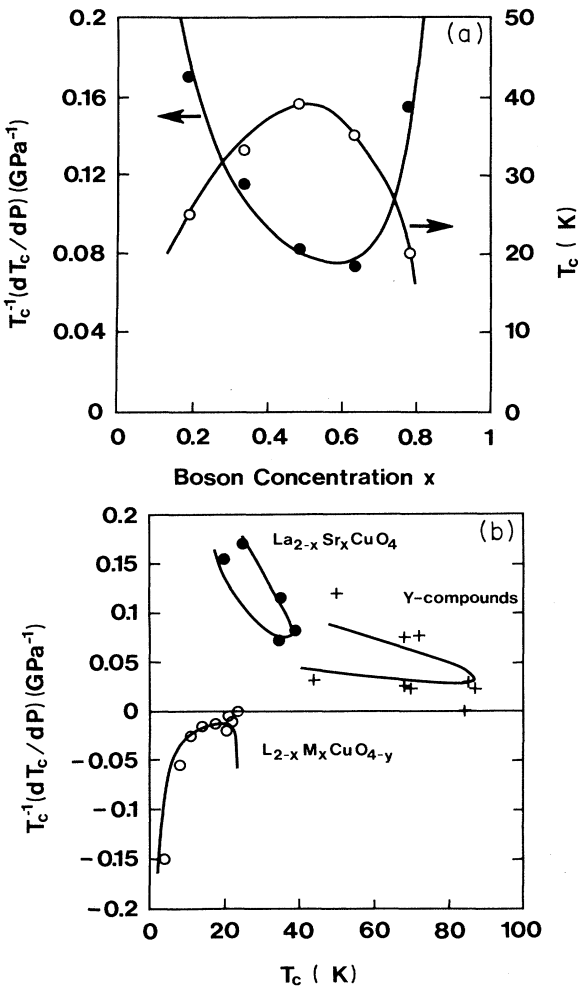

FIG. 6. (a) Comparison of the experimental pressure effect (solid circles) for $La_{2-x}Sr_xCuO_4$ with the estimation of the theoretical model. (b) The pressure derivative D of the logarithm of T_c as a function of T_c. Theoretical results (solid lines) are calculated from Eq. (23) with the fermion mass equal to $0.07m_e$ and the boson mass $2m_e$, and the density parameter r_0=3.65, 3.3, and 2.7 for $La_{2-x}Sr_xCuO_4$, the Y-based compounds and the electron-doped compounds, respectively. The experimental data are from Ref. 54 for $La_{2-x}Sr_xCuO_4$, Ref. 37 for the Y-based compounds and Ref. 38 for the electron-doped compounds $L_{2-x}M_xCuO_{4-y}$. Notice that only the data for the Y-based compounds from Ref. 37 are included for the sake of clarity. In (a) the corresponding critical temperatures T_c are shown by open circles.

efficient D will change sign in the region $0 \leq x_B \leq 1$, although one now needs a more detailed model for the quantity $\bar{\kappa}$ in Eq. (24). In any case this would be a model where the holes are divided into "superconducting" and "nonsuperconducting" ones, a model rejected in the early days of superconductivity.

V. EVIDENCE FOR THE ELECTRON COMPONENT: SPECIFIC HEAT

It has now become increasingly evident[23–27] that the high-T_c compounds at low temperatures do have a linear term, which we take to be the sign of the existence of mobile electrons in these compounds. Other evidence[55] comes from the ultrasound attenuation which does not show a discontinuous drop at T_c observed for ordinary BCS superconductors. The main argument in the BCS case is that in normal metals at low temperatures the ultrasound is absorbed mainly by mobile electrons. At T_c they go into the forming of Cooper pairs and hence the attenuation drops suddenly. With the present approach the observed behavior can be understood in terms of the electrons which continue to coexist with the superconductivity for $T < T_c$, and nothing much happen at T_c. As discussed in the Introduction the drop should more likely occur at $T_{\rm BCS}$.

At this time there is still no direct evidence about the existence of the electron sound mode proposed in Ref. 3. Indirect evidence comes from the Raman experiments which show a continuous spectrum inside the gap.[56] In addition the pair-breaking spectrum at 2Δ in Raman scattering is not visible as it is in the case of BCS superconductors. In this respect the situation is similar to the one in ultrasound attenuation. Clearly the wave function Eq. (18) of the EHBL model would produce a continuous spectrum in the gap.

Yet another experiment where the effect of the BCS gap at T_c is not seen is the infared absorption. The experimental evidence supports the idea that midinfrared absorption is a direct electronic excitation,[57] again supporting the EHBL model.

Direct proof for the existence of electron sound would come from Brillouin scattering. In addition to the normal acoustic modes one should see an extra longitudinal mode below T_c but not above $T_{\rm BCS}$. With neutrons, on the other hand, only the crystal modes should be visible. In compounds like $La_{2-x}Sr_xCuO_4$ the sound velocity should behave according to Fig. 3 as a function of x in doping. The speed u_e is close to the Fermi velocity corresponding to the electron density n_e.

The main evidence for the existence of electrons in the superconducting state comes from the linear term in specific heat at low temperatures. Since the bosons contribute a cubic term one can write the specific heat at low temperatures in the form

$$c = \gamma(0)T + \gamma_3 \left(\frac{k_B T}{\hbar u_e}\right)^3 + \gamma_L \left(\frac{k_B T}{\hbar u}\right)^3 . \tag{26}$$

The lattice part can in principle be determined by the measurements above T_c but no data exist for a single specimen all the way from $T > T_c$ down to $T \sim 0$, accurate enough to enable one to separate out the lattice part. Accurate determination of the average lattice velocity u would also enable one to determine the value of u_e. In the most simplified theory, $\gamma(0)$ is given by the same expression as for normal metals

$$\gamma(0) = k_B^2 m_e^* k_F / 3\hbar^2 . \tag{27}$$

This assumes a spherical Fermi surface which is perhaps too idealized for such complicated lattices. Microscopically the electron-hole excitations would enter in $\gamma(0)$. The coefficients γ_3 and γ_L are given by

$$\gamma_3 = 2\pi^2 k_B/15 , \quad \gamma_L = 3\gamma_3 . \tag{28}$$

At higher temperatures $T \leq T_c$ the existence of the Brillouin zone structure also for the k vectors of electronic excitations would suggest a kind of Debye model for the electronic part as well. The γ_3 term would then be a low-temperature limit of such an expression. The simplest way to proceed is to allow for u_e a slight temperature dependence. The numerical model calculations show that the sound mode dispersion develops a plateau before cutting into the particle-hole continuum as is also evident from Fig. 3. This plateau lies orders of magnitude higher than the gap[17] $\approx (2\text{–}8)k_B T_c$. Similar structure will evidently occur at much lower energy due to the pair-breaking excitations. We anticipate that this crossing together with fluctuations can cause sharp temperature variation of the sound velocity near T_c, similar to the one occurring in He mixtures near T_λ. Effectively this will be reflected as a sharp temperature variation of the coefficient a_3 in the specific heat. We can proceed to analyze the situation near T_c in the light of He mixtures and allow temperature dependence for u_e.

A useful way to analyze the jump of the specific heat at T_c is to calculate the normalized slope[30,31]

$$R = T\frac{d}{dT} \ln \Delta c \Big|_{T=T_c} , \tag{29}$$

where $\Delta c(T)$ is the difference between the superconducting and the normal state. If we allow some modification of the cubic term in Eq. (26) at elevated temperature near T_c due to the effects discussed above we may use the following form for $c(T)$:

$$c(T) = \gamma(0)T + a_3(T)T^3 + c_L(T) . \tag{30}$$

The discontinuity in the slope is then given by the second term in Eq. (30), the lattice term c_L and the linear term are supposed to have continuous derivatives at T_c, therefore the normalized slope is given by

$$R = 3 + T_c \frac{d}{dT} \ln a_3 \Big|_{T=T_c} = 3 - 3T_c \frac{d}{dT} \ln u_e \Big|_{T=T_c} . \tag{31}$$

The experimental results[30] for R scatter between 8 and 25. The maximum value for R obtainable from Eliashberg theory[31] is 5 and the BCS theory gives R=2.6. In order to reach the experimental values with the present model using Eq. (31), the electron sound velocity u_e should diminish strongly with temperature near T_c within a small temperature interval. Since present theory is closely related to the case of superfluid He mixtures, many features known from there should also apply here. It is well known that[43] in these mixtures the nature of the discontinuity in the specific heat depends in a sensitive way upon the concentrations and the pressure. In pure He the derivative of the first sound velocity has a dip.[58] For the He mixture[59] the feature fades away with increasing ^{3}He concentration.

To take an example, let us suppose that near T_c also in the high-T_c superconductors the sound velocity gets diminished by the following exponential law:

$$u_e(T) = u_0(1 - \beta e^{-\alpha t}) , \quad t = 1 - T/T_c , \tag{32}$$

for $T < T_c$. Then, if β is small, we obtain

$$R = 3 + 3\alpha\beta . \tag{33}$$

Suppose further that the maximum variation of u_e is 5% which occurs within 2 K for $T_c \approx 100$ K, we then obtain β=0.05, α=100, and R=18. Clearly Eq. (32) and the numbers obtainable from there are purely illustrative, but it shows that large values of R can be understood within the present approach.

Our final remark concerns the dependence of the low-temperature specific heat upon pressure and magnetic field. To our knowledge no direct measurement of the pressure dependence of the specific heat exists. In Ref. 60 it was found that the linear term was increased and the cubic term decreased in high magnetic field at low temperatures. Applying the available theories there, this experimental result remained unexplained.[60] Our explanation would start with the assumption that the main effect of external magnetic field would be the compression of the specimen. We know from the pressure dependence discussed in Sec. IV that n_e, n_B, and u_e would all increase. Therefore $\gamma(0)$ would increase as k_F and γ_3 would decrease. The relevant formulas for the coefficients $\gamma(0)$ and a_3 of Eq. (30) are simply

$$\frac{\partial \ln \gamma(0)}{\partial P} = \kappa_e/3 ,$$
$$\frac{\partial \ln a_3}{\partial P} = -3n_e\kappa_e \left(\frac{\partial \ln u_e}{\partial n_e} + \frac{1}{2}\frac{\partial \ln u_e}{\partial n_B} \right) . \tag{34}$$

The gradient of $\gamma(0)$ is determined by the electron gas compressibility, and using the notations of Eq. (23) the gradient of the cubic term can be written in the form

$$\frac{\partial \ln a_3}{\partial P} = -\kappa_e \left(1 + \frac{3M(1-2\mu)}{4(4\mu^2 + M\mu)} + \frac{c' n_e^{1/3}}{2(1 + c' n_e^{1/3})} \right) . \tag{35}$$

This is always negative. Unfortunately we do not know the relation between the hydrostatic pressure and the magnetic field to be able to make a comparison with the experiment, but we can at least understand the signs. As was discussed in Sec. IV the signs of the pressure gradients would be opposite for electron-doped superconductors.

VI. DISCUSSION

What can be said about various parameters of the high-T_c superconductors in the light of the theory presented here? Unfortunately not very much as yet because the temperature dependence is still not accurately done, various correction terms are difficult to evaluate, and because u_e has to be obtained from the Euler-Lagrange equation by numerical calculations. The effect of nonisotropy can also be large. Nevertheless we find it useful to recollect here the most relevant quantities one may start using in order to extract information about densities n_e, n_B, the effective masses $m_e^* = \mu_e m_e$ and $m_B^* = \mu_B m_e$, the Landau points x_1 and x_2, and the factor $\Gamma(n_e, n_B)$. We start by recollecting formulas from preceding sections in the following form:

$$T_c = 61.3 \left(\frac{100}{r_0} \sqrt{\frac{\Gamma}{\mu_e}} \right)^2 \left(\frac{\mu_B x \Gamma}{\mu_e} \right)^{1/4} (1-x)^{5/12} \text{ K} , \tag{36}$$

$$u_e = 4.20 \times 10^6 \Gamma (1-x)^{1/3}/r_0\mu_e \text{ m/s} , \tag{37}$$

$$\gamma(0) = 19.7\mu_e(1-x)^{1/3}/r_0 \text{ mJ/K}^2 \text{ mol} , \tag{38}$$

$$\frac{\partial \ln T_c}{\partial P} = \left(\frac{5}{12} + \frac{7}{16\mu} - \frac{5}{8}\frac{(2+\mu)}{(4\mu + M)} + \frac{5}{24}\frac{c'(1-x)^{1/3}}{1 + c'(1-x)^{1/3}} \right) \kappa_e \text{ GPa}^{-1} , \tag{39}$$

$$\kappa_e = [r_o\mu_e/6.13(1-x)^{1/3}]^5 \text{ GPa}^{-1} . \tag{40}$$

The most inaccurate of these is perhaps the formula for T_c of Eq. (36), partly because the linear spectrum cannot be correct all the way up to T_c. The main source of inaccuracy, however, is in the sound velocity u_e which should be determined by experiment or numerical calculation with the Euler-Lagrange equations and not simply from Eq. (37). Therefore the determination of the parameters at this stage may not be meaningful. The pressure formula would require the density parameter r_0 to be approximately 3.6. The best fit for the pressure curve gives $m_e^* \approx 0.1 m_e$ and $m_B^* \approx 2m_e$. This assumes that the correction term in the T_c formula is a nearly constant, multiplicative factor. The simplest way to estimate the effect of the depletion of the Bose condensate by hole pairs is to replace the boson density n_B in Eq. (19) by $\eta(T_c, T_{\text{BCS}})n_B$. At the present we do not know

whether η can be taken from the BCS theory or from its two-dimensional variant. In any case it will give a multiplicative factor < 1 and hence not change our theory in a major way. The reduction factor η will depend upon the way the crossing of the sound mode and the pair breaking takes place. In liquid He the phonons alone would give[2] $T_\lambda \approx 7$ K, and only after adding the roton contribution it comes down close to the experimental value. Furthermore near T_λ roton-roton interactions become important there.

With reference to the picture given in the Introduction, we have presented evidence that within the present model one can understand at least qualitatively many experimental findings. The solution of the central problem of the exact binding mechanism of the pairs is not attempted in any way here. However, since our model predicts a crossing of the pair-breaking excitation and the sound mode, some understanding of the binding mechanism is needed in the continuation, likewise the behavior of the sound mode at Landau damping point x_1 and x_2 needs more study. In principle the model can readily be generalized to a lattice but one no longer can work with analytical expressions as was done here.

In the present paper we have not discussed the resistivity, magnetic properties, Raman experiments, and NMR. We believe that in the two former ones the nonisotropy plays a major role. For the Raman experiments we predict the existence of a continuum spectrum in the gap which is also observed. In the case of NMR we can present only some very preliminary ideas. Clearly our model would predict linear temperature behavior for the relaxation rate near $T=0$. This linear term should be there for the same reason as in the case of specific heat: due to the free electrons. This seems to agree with some experiments.[61] Correspondingly in the Knight shift at $T=0$, part of the "orbital" shift can be interpreted as a constant shift due to the electrons which in BCS do not exist.[62] We therefore predict an approximate Korringa relation for the relaxation rate T_1^{-1} for the plane Cu(2) at low temperatures. At elevated temperatures $T < T_c$ the superfluid part of the Knight shift would follow a $(T/T_c)^4$ behavior up to T_c. This would predict a $(T/T_c)^5$ behavior[63] for T_1^{-1} below T_c with no shoulder.[62] The shoulder should be visible at $T_{\rm BCS}$ but the structure does not need to be BCS-like. For Cu(2) such a shoulder appears to be present[61] in $YBa_2Cu_4O_8$ at 500 K which is another fact in favor of existence of $T_{\rm BCS}$ at this temperature. Depending upon the mechanism of binding for the hole pairs the present model can predict nonmetallic behavior for $T_c < T < T_{\rm BCS}$ in NMR.

For elements situated outside the CuO_2 planes the superfluid contribution to the Knight shifts comes from the collective sound mode. The Korringa relation seems to be valid in some experiments for the nonplane elements[61] below T_c. This again is due to the mobile electrons. In Ref. 63 for the Cu(2) site the Knight shift was shown to be constant in temperature when $\mathbf{H} \parallel$ c. This we interpret to mean that the superfluid density vanishes at the Cu(2) sites but the electrons can travel through the CuO_2 planes at these points and the bosons are situated at plane sites O(1). This would be in agreement with our annihilation argument. The real pair-breaking effect for $T > T_c$ in the Knight shift should only be seen for O(1) sites in NMR for ^{17}O, which is also found[64] in $La_{1.85}Sr_{0.15}CuO_4$. For this compound $T_{\rm BCS}$ would be the point where this Knight shift becomes constant, which happens at $T \approx 270$ K.

In conclusion, we make the following points: (1) our EHBL model proposes the existence of electrons and hole bosons as mobile charge carriers. (2) Such a mixture exhibits a collective electron sound mode. The speed of the electron sound is of the order of magnitude of the Fermi velocity corresponding to the electron density n_e. (3) At T_c essentially a normal λ transition takes place. (4) The electronic specific heat contains a linear term due to the electrons and a cubic term due to the electron sound mode. (5) The asymmetry in the pressure dependence of T_c for electron-doped and hole-doped superconductors is in agreement with experiment. In both cases the effective mass required for the fermion component is roughly one-tenth of an electron mass whereas the boson mass is larger than $2m_e$. In both cases we make a definite prediction for the pressure dependence of specific-heat coefficients $\gamma(0)$ and a_3. (6) Within the present model the normalized slope of the specific-heat discontinuity at T_c can reach the experimental values which are found to be larger than the ones predicted by BCS and Eliashberg theories. (7) The existence of the sound mode can be experimentally confirmed by Brillouin scattering. Besides the Brillouin scattering experiments we would still need new specific-heat data, done with a single specimen, all the way from $T \approx 0$ to $T > T_c$, to enable one to separate out the lattice part. (8) Some features of NMR can be readily understood.

ACKNOWLEDGMENTS

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