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Are the New High Temperature Superconductors Strong Coupling Systems?*

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ABSTRACT

Under certain circumstances the excitations of a superconductor will not be those predicted by BCS theory, but rather *electron bag* states. A variational calculation is used to establish this regime in which such collective states form. The fact that such bags may bind more than one electron implies the existence of more than one peak in the plots of dI/dV versus V_P obtained in Giaver tunneling experiments. The estimate of the number and ratios of voltages associated with such peaks is in qualitative agreement with recent experimental results.[3]

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Speculation that the new high temperature superconductors[1] are strongly coupled systems has been widespread. The strong coupling behavior of BCS-like systems is not commonly discussed in solid state physics, but it has been looked at extensively in particle physics.[2] The purpose of this letter is to present some simple results which follow from applying such ideas to the new class of superconductors. This analysis implies striking differences between the behavior of these superconductors and the more familiar weak coupling superconductors studied in BCS theory; this behavior appears to have been seen in the Giaever tunneling experiments carried out at Stanford by Smith *et.al.*[3]

In superconducting systems, due to their interaction with the condensate, fermions above the fermi surface behave as massive particles. Under certain circumstances an extra fermion injected into the system can lower its mass by expelling condensate from its immediate neighborhood. It will then produce a region, or *bag*, of radius R, filled with normal material and trap itself in this region. Such objects have been discussed for the case of quantum field theory in the context of the SLAC bag model of hadrons.[2]

To decide whether such an excitation has a lower energy than the energy of a single electron as computed in BCS theory, it is necessary to obtain an upper bound on the energy of a one-electron bag. This bound depends upon the *condensation energy*, which determines the energy required to drive a spherical region normal, and the energy which required to localize the extra electron inside the normal region. The question is for what range of parameters will the energy of the *one-electron bag state* be smaller than the gap Δ_0. When this happens, the BCS description of the lowest lying excitations must break down.

The starting point of the argument is the familiar BCS Hamiltonian

$$H = \sum_{\vec{k}} \epsilon_{\vec{k}} c^{\dagger}_{\vec{k}} c_{\vec{k}} + \sum_{\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4} V_{\vec{k}_1\vec{k}_2\vec{k}_3\vec{k}_4} c^{\dagger}_{\vec{k}_1} c^{\dagger}_{\vec{k}_2} c_{\vec{k}_3} c_{\vec{k}_4}$$

where the usual simplification is to assume that $V_{\vec{k}_1\vec{k}_2\vec{k}_3\vec{k}_4} = -V\delta_{\vec{k}1,-\vec{k}_2}\delta_{-\vec{k}_3,\vec{k}_4}$ for $|\epsilon_{\vec{k}_i}| < \hbar\omega_D$, and zero otherwise. The usual BCS calculation is equivalent to a variational calculation wherein we choose as a trial state the ground state of a quadratic Hamiltonian with a constant mass M. The minimization of the expectation value of the BCS Hamiltonian as a function of the mass parameter, M, yields the BCS gap $M = \Delta_0$. The condensation energy, $\Delta\mathcal{E} \approx n(0)\Delta_0^2/4$, is the difference between the expectation value of the BCS Hamiltonian in the state corresponding to $M = 0$ and that for $M = \Delta_0$. Here, $n(0)$ is the density of states near the Fermi surface. To obtain an effective quadratic Hamiltonian for the electrons we replace the operators $c^{\dagger}_{\vec{k}_1} c^{\dagger}_{\vec{k}_2}$ or $c_{\vec{k}_3} c_{\vec{k}_4}$ by their constant expectation values in the trial state. This yields a Hamiltonian for a fermionic excitation of mass Δ_0.

To calculate the energy of a *baglike* excitation we follow the same reasoning, but do not assume that the expectation value is translationally invariant. Rather, we assume that it has the form shown in Fig 1. In that case the electron's contribution to the bag energy is obtained by solving for the lowest eigenstates of a quadratic fermionic Hamiltonian with a position dependent mass term. A complete analysis of this problem for the analogous field theory problem is given in Ref. 2.

For the s-wave states it costs an energy of order $1/R$ to put an electron into the lowest eigenstate of the bag (for the moment we ignore Coulomb effects); the

cost of putting an electron into the first state with one node is approximately $2/R$. Making these approximations, we see that for a single electron in a bag, the quantity

$$E_1(R) = (4\pi/3)[n(0)\Delta_0^2 R^3/4] + (1/R) \tag{1}$$

provides an upper bound on the energy of the lowest-lying baglike state. We should, in reality, include a term of the form dR^2 to represent the energy due to the transition region in which the groundstate expectation value of the condensate changes from zero to its bulk value (d stands for the width of the transition region as shown in Fig.1). While this term is easy to obtain for the field theory case it is more difficult to obtain from the BCS approximation. In order to present the argument in simplest terms we will initially ignore the presence of such a surface term. Minimizing Eq(1) with respect to R yields

$$R^{-1} = (\pi n(0)\Delta_0^2/3)^{1/4} \quad ; \quad E_1 = (4/3)(\pi n(0)\Delta_0^2/3)^{1/4}. \tag{2}$$

The condition that the *one electron bag* lie lower in energy than Δ_0 is

$$(4/3)[\pi n(0)/3]^{1/4} < \Delta_0^{1/2}. \tag{3}$$

This suggests that if we use Eq. (3) as a definition of strong coupling, then such a system should be characterized by a small density of electrons available for pairing.

Since the first electron has already paid the price for creating a bag, what happens if we place another electron in the same region? Since the second electron can fall into the same spatial wavefunction, because the spins can anti-align, for

such a two-electron bag, we have

$$E_2(R) = \pi n(0)\Delta_0^2 R^3/3 + 2/R \tag{4}$$

which, at the minimum, is

$$E_2 = 2^{3/4} E_1 \tag{5}$$

Since the energy of two separate one-electron bags is $2E_1$, we see that the physics of a strong coupling condensate causes a localized, doubly charged, spin zero bound state to form. In other words, the interaction between two localized one-electron bags will be attractive.

If we now attempt to add a third electron to the bag we can no longer put it into the s-wave bound state. We can, however, put it into a state with a single node, increasing the localization energy by an additional term of $2/R$. Thus the energy of the localized three-electron bag is given by

$$E_3(R) = [\pi n(0)\Delta_0^2 R^3/3] + [(1+1+2)/R] \tag{6}$$

and so at the minimum we have

$$E_3 = 4^{3/4} E_1 \tag{7}$$

Since $4^{3/4} > 1 + 2^{3/4}$, we see that for a bag energy which doesn't include a surface term the interaction between localized two and one-electron bags is repulsive.

Thus, in the strongly coupled system, unlike the ordinary weak-coupling BCS approximation, there are two distinct sets of levels available for the tunneling of electrons *into* the superconductor. Hence, in Giaever tunneling into a sample of

this kind of superconductor, one would expect the plot of dI/dV to show two peaks at distinct values of V_P. This result is the most important qualitative feature which distinguishes the strong coupling superconductor, as we have defined it, from ordinary weak coupling superconductors which are well described by the usual BCS analysis. Note, such distinct states may not be readily available as sources for taking electrons *out* of the superconductor, which would imply asymmetrical behavior in Giaever tunneling experiments. Whether or not this has anything to do with the asymmetry seen in the Stanford tunneling experiments awaits to be seen. To calculate the location of these peaks one has to refine this calculation; however, before doing this we should first return to the question of the surface energy term in $E(R)$ and the question of including the Coulomb force.

In general the cost of creating a localized normal region will be described by both a volume and surface term. Thus, we expect the energy of a one-electron bag to have the form

$$AR^3 + BR^2 + 1/R \tag{8}$$

There are two extreme cases; $A = 0$ and $B = 0$. We have already discussed is the $B = 0$ case. Also, since the electrons are charged, localizing them inside the bag will cost Coulomb energy. Since these particles are in quantum states which are more or less uniformly spread out over the radius of the bag, gives a contibution to $E(R)$ of the form xn^2/R; where n stands for the number of electrons in the bag and the parameter x is a factor introduced in order to absorb shape and wavefunction factors that do not calculated in this approximation. The general expression for the energy of such a one-electron bag state is therefore:

$$E(R) = AR^3 + BR^2 + (1 + x)/R \tag{9}$$

If $B = 0$, the one-electron energy will be proportional to $A^{1/4}(1+x)^{3/4}$. If on the other hand $A = 0$, the one-electron bag energy is $B^{1/3}(1+x)^{2/3}$. If this energy is less than the Δ_0 obtained from the BCS calculation, then we have *prima facie* evidence for the fact that the BCS description of the excited states of the superconductor has broken down.

We can carry out the calculations for multi-electron bags for both limits. The results for $B = 0$ are

$$\begin{aligned} E_1 &= A^{1/4}(1+x)^{3/4} \quad ; \quad E_2 = [(2+4x)/(1+x)]^{3/4}E_1 \\ E_3 &= [(4+9x)/(1+x)]^{3/4}E_1 \quad ; \quad E_4 = [(6+16x)/(1+x)]^{3/4}E_1 \end{aligned} \tag{10}$$

The results for $A = 0$ are

$$\begin{aligned} E_1 &= B^{1/3}(1+x)^{2/3} \quad ; \quad E_2 = [(2+4x)/(1+x)]^{2/3}E_1 \\ E_3 &= [(4+9x)/(1+x)]^{2/3}E_1 \quad ; \quad E_4 = [(6+16x)/(1+x)]^{2/3}E_1 \end{aligned} \tag{11}$$

We see that there is a crucial difference between these two cases, since in the case $A = 0$ there exists an additional three-electron bound state. All bags containing more than three electrons are unbound in both cases.

These results imply that Giaver tunneling experiments will show either two or three peaks, depending upon the specific properties of the superconducting sample. Since the present perovskite superconductors are multi-phasic materials it is entirely possible that both kinds of behavior will be seen. It is not clear whether or not such a difference has in fact been observed.[3]

While this result is suggestive, one has to be careful to observe that to this point the calculations are for localized bag states. If a localized state exists, then translating the center of the bag by an arbitrary amount yields a configuration

having exactly the same energy. To calculate the lowest energy bag state one must calculate the expectation value of the Hamiltonian in such a plane wave state; such a calculation of this type is difficult, and lies outside the scope of this paper. We can estimate the effect if we consider the kinetic terms (which allow for the mixing of shifted bag states) as perturbations of the energy. Since the kinetic terms are bilinears in the fermion operators they can move a one-electron bag in first order, a two-electron bag in second order, etc. If the typical strength of such a *hopping term* is represented by a parameter $A^{1/4}g$ or $B^{1/3}g$, then we might expect ratios of multi-electron bag states to the one-electron bag state to be

$$E_{2/1} = [(2+4x)^{\frac{3}{4}} - g^2]/[(1+x)^{\frac{3}{4}} - g];\ E_{3/1} = [(4+9x)^{\frac{3}{4}} - g^3]/[(1+x)^{\frac{3}{4}} - g]$$
$$E_{4/1} = [(6+16x)^{\frac{3}{4}} - g^4]/[(1+x)^{\frac{3}{4}} - g] \tag{12}$$

for the case $B = 0$, and

$$E_{2/1} = [(2+4x)^{\frac{2}{3}} - g^2]/[(1+x)^{\frac{2}{3}} - g];\ E_{3/1} = [(4+9x)^{\frac{2}{3}} - g^3]/[(1+x)^{\frac{2}{3}} - g]$$
$$E_{4/1} = [(6+16x)^{\frac{2}{3}} - g^4]/[(1+x)^{\frac{2}{3}} - g] \tag{13}$$

for the case $A = 0$. Ratios, rather than absolute energies are calculated in order that unknown factors cancel out. Tables I and II present the results of computing these ratios for various values of g and x. Since the factors of $1/R$, $2/R$, etc, are obtained by assuming that the wavefunction of the electron vanishes at the walls of the bag, it is possible that a more careful analysis taking the finiteness of Δ_0 into account could lead to a third bound state for the three-electron bag. For this reason the ratio to the three-electron case is included in the case $B = 0$ because it is only marginally unbound. While the present calculation does not support this

possibility display the prediction for the three-electron bag as if it was bound in order to exhibit the sensitivity of the ratios to the various assumptions. Tables I and II show that the ratios do not change all that much between the extremes $A = 0$ and $B = 0$; the results for intermediate cases lie in between. Note, the higher states, once the kinetic terms are taken into account presumably represent resonances and not true eigenstates of the full Hamiltonian.

The dI/dV curves of Smith *et.al.* for both the LaSrCuO and YBaCuO type superconductors, clearly exhibit more than a single peak. Data at different points on the sample exhibit slightly different ratios for the locations of the peaks and not all the points exhibit three peaks. This could imply that the different regions correspond to phases with different values of the parameters A, B and g. Were all samples to exhibit three peaks with ratios of 1:3:5, this would favor a surface dominated bag with $g \approx .53$.

To conclude, staying within the context of a BCS theory, it has been argued that the charged excitations of the strong coupling theory will not be the fermions of the BCS solution, but will instead be collective excitations. The number of excitations of this type will be finite, most likely two or three in number and should show up as peaks in the dI/dV plots obtained in Giaever tunneling experiments. Furthermore, it is entirely possible that the structure seen when one tunnels electrons into the superconductor can be different from what is seen going the other direction. It is much more difficult to compute the relation of the critical temperature to the gap, since in order to do the calculation correctly the effect of these extra states must be taken into account. Most likely it will be necessary to redo the BCS calculation in order to obtain a correct prediction. Techniques which have been applied to analogous problems in particle physics

may be useful for this calculation.

From an experimental point of view, there is one interesting feature of this class of excitations that might be tested; namely, that the states of the bag which correspond to radial excitations of non-zero angular momentum can be split in a magnetic field. Since these materials are type II superconductors, at high field there are many flux tubes penetrating the material. Hence, if a sample is placed in a strong magnetic field, and if the penetration depth of the field into the superconducting volume is large enough, then the number of bound states which can exist in a bag may change because states which are degenerate at zero field now split. It would be interesting to measure dI/dV for these materials as a function of applied magnetic field.

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Table I(a):volume dominated $x = 0$			TableI(b): $x = .03$	
g	E_2/E_1	E_3/E_1	E_2/E_1	E_3/E_1
.4	2.54	4.61	2.57	4.67
.42	2.60	4.75	2.62	4.80
.44	2.66	4.90	2.68	4.95
.46	2.72	5.06	2.75	5.10
.48	2.79	5.14	2.81	5.27
.50	2.86	5.41	2.88	5.45

Table II(a): surface dominated $x = 0$			Table II(b): $x = .03$	
g	E_2/E_1	E_3/E_1	E_2/E_1	E_3/E_1
.47	2.58	4.56	2.60	4.60
.49	2.64	4.71	2.66	4.74
.51	2.71	4.87	2.73	4.90
.53	2.78	5.04	2.80	5.07
.55	2.86	5.23	2.87	5.25
.57	2.94	5.43	2.95	5.44

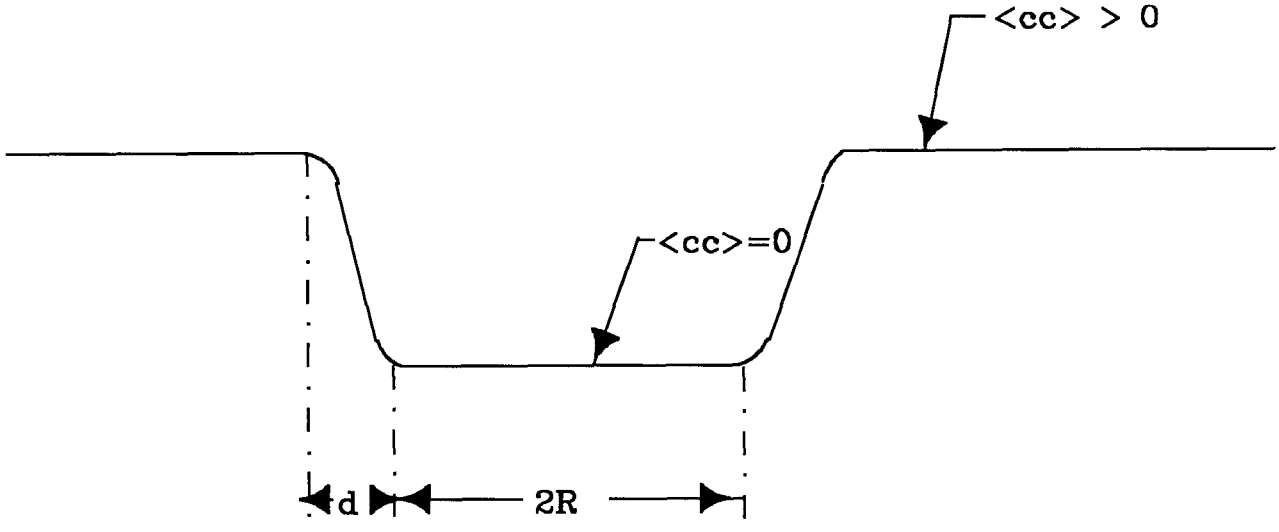

Fig. 1