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Bosonic Mechanism for High Temperature Superconductors

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The temperature dependent photoemission data of D.S. Dessau *et al.*[1] show strong modulations in the superconducting state when compared to the normal state. These are similar to but larger than those seen historically in standard tunneling experiments in lower temperature superconductors. We have analyzed the Dessau data using Nambu-Eliashberg theory assuming some (as yet unknown) boson exchange as the primary mechanism for the superconductivity.[2] The derived α^2F's, λ's and μ^*'s show features which resemble those derived from inversions of other low-temperature superconductors, albeit that λ here is about 8.67 and μ^* is approximately 0.15. Several bosonic mechanisms are considered.

Temperature dependent angle-resolved photoemission experiments, although very different from tunneling in the laboratory environment in terms of techniques, probe similar physics close to the fermi level E_F. Both effects are proportional to the electron density of states. A major difference is that phtoemission data only sense electrons from below E_F, whereas through biasing, tunneling experiments sense density of states structure both above as well as below E_F. We show in Fig. 1 a long count photoemission run of Dessau *et al.*[1] taken along the (110) direction, near the Fermi surface. It is tempting to apply Nambu-Eliashberg (NE) theory to these data.

The typical energy resolution of photoemission data is about 10-15 meV, whereas that of tunneling data is better than perhaps 0.1 meV. Hence in applying NE theory to photoemission data we need to take into account a broader spectral resolution function in some detail. In Fig. 2 we show as the open squares a plot of

$$g(E)^{exp} = \frac{\sigma_s(E)}{\sigma_n(E)} - 1 \quad , \tag{1}$$

where $\sigma_s(E)$ is the 20 Kelvin data of Fig. 1, and $\sigma_n(E)$ is the 100 Kelvin data extrapolated as the dashed line in Fig.1. One can see that $g(E)^{exp}$ has strong coupling modulations, similar to those $g(E)$'s derived from tunneling data of conventional superconductors such as Hg or Nb.[3,4]

We have solved numerically the Eliashberg nonlinear coupled integral equations derived from the two components of Nambu's iso-spin equations[5,6] in which we have explicitly preserved their nonlinearity. Because the broadening of the experimental data is large in comparison to tunneling data, a direct inversion along the lines of references (6) and (8) is not feasible. Instead, we adopt the approach described below

The superconducting density of electron states N(E) is given by

$$N(E) = Re\left\{\frac{E}{\sqrt{E^2 - \Delta^2(E)}}\right\}, \qquad (2)$$

where $\Delta(E)$ is the τ_1 isospin component above. Equation 2 contains temperature broadening effects but no photoemission detector resolution effects. This density of states broadened by the experimental spectral resolution function $P(E, E')$ is what we take to be the theoretical $g(E)$ (plus one):

$$g(E)^{th} = \int_{-\infty}^{\infty} P(E, E')N(E')dE' - 1, \qquad (3)$$

This is the quantity to be compared in a least squares sense with the experimental data $g(E)^{exp}$ above. We have tried both Gaussian and Lorentzian forms for this resolution function.

For simplicity we approximate α^2F by a sequence of analytic functions[7] rather than using a conventional evenly-spaced numerical function. The broadening of the data is such that fine features in $\alpha^2F(E)$ are not directly reflected in it. Our goal is to determine the gross features in this function, leaving the calculation of finer features for the future. Details of our procedure will be given in a later paper. We show in Fig. 2 a typical $g(E)^{th}$ for a three-Lorentzian α^2F adjusted to fit the data.

We carry out a "double" variational procedure (in both resolution function and in α^2F), and we obtain the following:

In tunneling data on strong-coupling low T_c superconductors, it is known that the quantity we calculate is such that the location of peaks in $\alpha^2F(E)$ correspond to energies at which $|dg/dE|$ is peaked. In the present case, the substantial smearing of structure by limited experimental resolution (below, we find this resolution to be about 16 or 17 meV) makes such identification unreliable. In addition, we find that the lowest energy peak in α^2F (the only significant peak which we find) is at such a low energy that it falls quite close to the gap singularity. Indeed, the data are analogous to that for Hg,[3,4] where the gap is 0.83 meV and a large sharp peak in α^2F occurs at $E_P = 2meV$. The ratio $(E_p + \Delta_o)/\Delta_o$ is thus a little more than 3 for Hg. For our case, it is of order 1.5. In this sense, the data here are similar to an "extreme form" of Hg tunneling data.

One can see directly on looking at $g(E)^{exp}$ that this function drops much more rapidly with energy than does the BCS $g(E)$ just above the peak in g(E). This fast drop is an indication that there is a strong peak in α^2F at about this energy minus the gap energy.

The best fit is for Gaussian broadening (as opposed to Lorentzian broadening) with

$$\Delta_o = 18meV, \quad \sigma = 15.9meV, \quad \mu* = 0.15, \quad \lambda = 8.67, \quad \alpha^2 = 49.77meV \quad ,$$

and with the rms fit deviation devn = 0.135. Here σ is the standard deviation for the Gaussian, and α^2 is defined as the integral of $\alpha^2F(E)$ over all E.

The $\alpha^2F(E)$ function which produces the best fit is shown in Fig. 3. The sharp, dominant peak at 10 meV is striking. If this peak is shifted upward to 15 meV, we find devn increases to 0.488; so, obviously, the fit is very sensitive to the position of this peak. We can say, with high confidence, that such a peak must occur very near this energy for this choice of gap value. Changing the width of the 10meV peak or the value of the cutoff energy for $\alpha^2F(E)$ increases devn. The value of μ^* is less certain, but seems most likely to be between approximately 0.11 and 0.16. Changing the width σ of the resolution function or the gap Δ_o from the values given above also increases devn.

We find that the gap and μ^* are somewhat sensitive to the nature of the resolution function, while the position of the dominant peak in $\alpha^2F(E)$ is hardly changed at all. Because this peak position depends on the second zero-crossing, which is nearly invariant under the smearing operation, the invariance of the peak is as one would expect.

We conclude that our results with Gaussian broadening fit the data better than Lorentzian broadening. Our best fit has been included in Fig. 2 as the sequence of open squares for our preferred parameters. Our preferred $\alpha^2F(E)$ function and its parameters are shown in Fig. 3.

The coupling strengths, α^2, range between 45.3 meV and 51.8 meV for the Gaussian fits, and between 73.8 meV and 76.3 meV for the Lorentzian fits. These average coupling strengths are from 10 to 20 times larger than those which are typical of strong-coupling, low T_c superconductors such as Pb or Hg.

Our inversion of the photoemission data gives an energy gap at $T = 0$ of $\Delta_0 =$ 18 meV. This results in a ratio $2\Delta_0/k_BT_c$ of 4.6 for the experimental $T_c = 91K$ or of 5.2 for our calculated $T_c = 80K$. **IS CALCULATED Tc 80 OR 85?** How does this compare with energy gaps of $Bi_2Sr_2CaCu_2O_8$ measured by other means? The low-temperature gap of this material has been measured by a variety of techniques including far-infrared reflectance measurements of crystals of $Bi_2Sr_2CaCu_2O_8$ by Reedyk, *et al.*[5].

Applying a Kramers-Kronig analysis to their data, they obtained a real part of the conductivity that in the superconducting state has a sudden onset from a value at or near zero at a frequency of about 37.5 meV. Although these au argue that "the sharp edges in the superconducting reflectance are not necessarily energy gaps", we are struck by the fact that this onset at 37.5 meV is identical (within the errors of our inversion process carried out on the photoemission data with its limited resolution) with our 2 Δ_o = 36 meV.

Recent far-infrared transmission measurements on a single-crystal of $Bi_2Sr_2CaCu_2O_X$ with a T_c = $76K$ shows no energy gap,[9] but this can be understood by the fact that the high-temperature superconductors are near the clean limit. At the clean limit the gap is impossible to see by interaction with electronmagnetic radiation[9]. However more recent tunneling and far-infrared transmission measurements by this same group [10] on 2212 gives values of $2\Delta_o/k_BT_c$ of 7 to 12, "depending on the interpretation of the results."

A range of energy gaps have been reported from a number of tunneling measurements.[11,12,13,14,15,16,17,18] The ratio $2\Delta_o/k_BT_c$ runs from 3.4 to 8.7 (equivalent to from 13meV to 34meV for Δ_o), so that our gap of 18 meV falls in this range.

An energy gap $2\Delta_o$ of 58-60 meV was reported[19] using high resolution electron-energy-loss spectroscopy. This value is considerably higher than our value for the gap.

Two earlier photoemission measurements[20,21] were interpreted to give energy gaps $2\Delta_o/k_BT_c$ = 7 and 8 respectively, both values being considerably higher than our present value.

Results of recent femtosecond optical absorption studies[22] on high T_c superconductors also seem to indicate the existence of a sharp bosonic peak at low energies in these materials that interacts strongly with the charge carriers.

The large peak in α^2F at the low energy of about 10 meV leads to a large λ = 8.7. μ^* seems to be similar to that found for lower temperature superconductors, possibly indicating that Coulomb processes are similar in Bi 2212 to those of Nb_3Sn, but that λ is about four times larger. Direct numerical solution of the temperature dependent NE equations with these parameters produces a T_c of 85K. **IS CALCULATED Tc 80 OR 85?** Because of the large λ, it is perhaps questionable to employ the Dynes-Allen formula to calculate T_c. Nevertheless, we find, on using this formula with parameters derived from Gaussian broadening, the range of 61.5K to 72.6K for T_c with 65K for the best fit. All of these values are close to the experimental value of 92K for Bi 2212.

The sharp low-energy peak in Fig. 3 has a profound influence on the temperature-dependent resistivity in the normal phase. As has been discussed by Allen *et al.*,[23] one needs α^2F transport rather than our result in Fig. 3. We have assumed that the features of α^2F transport are similar to α^2F, but the overall magnitude may differ.

From λ alone, one can easily calculate the normal-state scattering lifetime and hence the temperature dependence of the resistivity in arbitrary units. We find that the resistivity is very nearly linear in temperature for temperatures above T_c. This is what is seen experimentally,[24] but can not be produced from models with Boson peaks at larger energies. To obtain the magnitude of the resistivity, we also need the Drude plasma frequency in addition to the electron lifetime.[23] Although the plasma frequency can be determined from infrared data, as pointed out in Ref. 25, "it is appropriate to be skeptical" of such determinations because various factors have to be subtracted from the data. We find it interesting that Allen *et al.*[23], after estimating λ to be less than one for both LSCO and YBCO, find that they cannot fit the magnitude of the experimental resistivity data. They conclude that one way they can fit this data is by "increasing λ by a factor of 5-10". Thus although they were considering different materials from BSCCO, they find that the resistivity data *may* be indicating that a large λ is required.

In summary, we have applied Nambu-Eliashberg theory to the Dessau *et al.*

photoemission data and have assumed that these (110) data are typical. The results of inversion produce a μ^* similar to that found in other superconductors and with a gap Δ_0 of 18 meV but with a λ near 8.7 and an α^2F with a large narrow peak at about 10 meV. Several types of Boson mediated mechanisms have been proposed for high-temperature superconductors including[25] acoustic plasmons, bi-excitons, and various forms of phonons. Any of these models can be consistent with a dominant peak at about 10 meV (120 Kelvin). If the large peak is due to phonons, such phonons would be strongly coupled to the electrons. Hence phonon lifetimes would be short, and phonon widths would be broad. We are unaware of any measurements of the phonon density of states derived, for example, from neutron scattering experiments for Bi 2212. Such experiments would be most helpful for comparison with our α^2F, and would tend to rule out, or support, phononic mechanisms. Large λ's have been considered before[26,27] in YBCO.

In this work work, we have considered photoemission data drawn from a small region of the Brillouin zone on the (110) line. We have assumed in peforming our inversions that this point on the Fermi surface is typical. The electronic band structure[28] suggests that these states are Bi rich, but that other points on the Fermi surface have different parentage. Hence it is possible that the gap, α^2F, and λ are in fact dependent on direction. This would necessitate a more complex inversion scheme than the one we have applied, but we believe that the main results of our work would remain intact. This also points toward the utility of experiments to probe anisotropies.

The (110) data are taken close to a place of band crossings; so it may be possible that the spectral features that we have analyzed are due to this band effect and not to strong coupling. One of us (FMM) has examined unpublished photoemission data of C.G. Olson[29] on Bi2212 searching for the band-structure possibility. We have concluded that the view we present here (the strong-coupling $\alpha^2 F$ model) is the more likely explanation of the Desseau *et al.* data.

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REFERENCES

1. Dessau, D.S., Wells, B.O., Shen, Z.-X., Spicer, W.E., Arko, A.J., List, R.S., Mitzi, D.B., and Kapitulnik, A. submitted for publication.
2. See also J.P. Carbotte's *Properties of Boson Exchange Superconductors, Review of Modern Physics* (in press).
3. Scalapino, D.J. in *Superconductivity* (ed. Parks, E.D.) Ch. 10 (Dekker, New York, 1969).
4. McMillian, W.L. and Rowell, J.M. *ibid*, Ch. 11.
5. Y. Nambu, *Phys. Rev.* **117**, 648 (1960).
6. E.L. Wolf and G.B. Arnold, *Physics Reports* **91**, 31 (1982).
7. J.R. Schrieffer, D.J. Scalapino, and J.W. Wilkins, *Phys. Rev.* **10**, 336 (1963).
8. M. Reedyk, D.A. Bonn, J.D. Garrett, C.V. Stager, T. Timusk, K. Kamaras, and D.B. Tanner, *Phys. Rev. B* **38**, 11981 (1988).
9. L. Forro, G.L. Carr, G.P. Williams, D. Mandrus, and L. Mihaly, *Phys. Rev. Lett.* **65**, 1941 (1990).
10. L. Forro, D. Mandrus, and L. Mihaly, preprint.
11. T. Hasegawa, H. Suzuki, S. Yaegashi, H. Takagi, K. Kishio, S. Uchida, K. Kitazawa, and K. Fueki, *Jpn. J. appl. Phys. Pt. 2* **28** L179, (1989).
12. S.I. Vedeneev, I.P. kazakov, S.N. Maksimovskii, and V.A. Stepanov, *Pis'ma Zh. Eksp. Teor. Fiz.* **4**, 588 (1988).

13. H. Ikuta, A. Maeda, K. Uchinokura, and S. Tanaka, *Jpn. J. Appl. Phys. Pt. 2* **27**, L1038 (1988).

14. M. Lee, D.B. Mitzi, A. Kapitulnik, and M.R. Beasley, *Phys. Rev. B* **39**, 801 (1989).

15. A. Th. A. M. de Waele, *et al.*, *Physica C* 153-155, 621 (1988).

16. Z. Shiping, *et al.*, *Solid State Commun.* **67**, 1179 (1988).

17. S. Vieira, *et al.*, *Phys. Rev. B* **38**, 9295 (1988).

18. T. Walsh, J. Moreland, R.H. Ono, and T.S. Kalkur, *Phys. Rev. Lett.* **66**, 516 (1991).

19. J.E. Demuth, B.N.J. Persson, F. Holzberg, and C.V. Chandrasekhar, *Phys. Rev. B* **64**, 603 (1990).

20. C.G. Olson, *et al.*, *Physica C* 162-164, 1697 (1989).

21. Y. Petroff, *Physica C* 162 164, (1989).

22. J.M. Chwalek, *et al.*, *Appl. Phys. Lett.* **57**, 1696 (1990); and submitted (1990).

23. P.B. Allen, W.E. Pickett, and H. Krakauer, *Phys. Rev. B* **37**, 7482 (1988).

24. D.B. Mitzi thesis, Stanford University (unpublished) (1989).

25. See for example, *High Temperature Superconductivity* (Addison-Wesley, NY, 1989), edited by K.S. Bedell, D. Coffey, D.E. Meltzer, D. Pines, and J.R. Schrieffer.

26. See for example, B.W. Veal *et al.*, *Physica C* **158**, 276 (1989).

27. V. Kresin (private communication).

28. S. Massidda, J. Yu, and A.J. Freeman, *Physica C* **152**, 251 (1988); H. Krakauer and W.E. Pickett, *Phys. Rev. Lett.* **60**, 1665 (1988); M.S. Hybertsen and L.F. Mattheiss, *Phys. Rev. Lett.* **60**, 1661 (1988).

29. C.G. Olson, (private communication).

FIGURE CAPTIONS

1. Temperature Dependence of Angle Resolved Photoemission Data of Bi 22112 taken along the (110) direction (After Reference 1). As discussed in the text these features resemble bosonic strong-coupling effects seen in lower temperature superconductors.

2. Experimental and theoretical values of the normalized "tunneling function" $g(E)$. The solid curve is the theoretical fit. The square boxes are derived from the data of Fig. 1. These features resemble those seen from tunneling in lower temperature superconductors.

3. Inverted $\alpha^2 F$ as a function of energy in meV. As discussed in the text, the sharp peak at 10 meV is the best resolved feature in this inversion.

~~4. The temperature dependent resistivity found from our preferred $\alpha^2 F$. The vertical line at 92 Kelvin marks the superconducting transition temperature.~~

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