WHAT DOES D-WAVE SYMMETRY TELL US ABOUT THE PAIRING MECHANISM?

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In this paper we argue that d-wave symmetry is a general consequence of superconductivity driven by repulsive interactions. Van Hove (or flat band) effects, deriving from the two dimensionality of the CuO$_2$ plane are important in stabilizing this state. By extending the original Kohn-Luttinger picture to a 2 D lattice, we find that the screened Coulomb term has important wave vector structure which leads to $d_{x^2-y^2}$ superconductivity.

There is a growing body of evidence to support the claim that the pairing symmetry in the cuprates is most probably d-wave, although some inconsistencies remain. These observations lead naturally to the question: what constraints does this information provide on the detailed nature of the pairing mechanism? In this paper we investigate this important question based on the Kohn Luttinger picture in which it was argued that the gap equation

$$\Delta_k = -\sum_{k'} V(k - k') \left( \Delta_{k'} \frac{\tanh \beta E(k')}{2E(k')} \right)$$

(1)

could be satisfied for repulsive interactions $V > 0$, provided $V$ contained some significant variation with wave-vector. A reasonable choice for $V(q)$ is the screened Coulomb interaction $V_{\text{eff}}(q, \omega) = V_0(q)/\epsilon(q, \omega)$ which in coordinate space exhibits the well known Friedel oscillations; thus there are regions of negative sign and superconductivity can take advantage of this attraction by forming anisotropic Cooper pair states.

The magnetic pairing scenario, which has been widely discussed for the cuprates, may be viewed as a simple extension of the Kohn Luttinger picture where the repulsive interaction (in wave vector space) is chosen to be the magnetic susceptibility with peaks around the $(\pi/a, \pi/a)$ point. As was shown by several different groups, this particular form for the wave-vector dependence in $V(q)$ leads to a $d_{x^2-y^2}$ pairing symmetry.

While this scenario evidently explains the pairing symmetry, it is not at all clear whether it is the appropriate mechanism for the superconductivity in the cuprates. Our group has extensively investigated this question based on the constraints imposed on the magnetism by neutron data in the copper oxides, and have inferred that the magnetism appears too weak to be responsible for the high superconducting transition temperatures found in the cuprates.
Where, then, does the $d_{x^2-y^2}$ symmetry originate? To address this question we first build intuition by analyzing a simple “generic” model which contains variable wave vector structure. This wave vector structure is crucial for anisotropic superconductivity. Consider $V(k_x, k_y)$ given by

$$V(k_x, k_y) = \frac{\lambda}{[1 - J_o(\cos(k_x \pm Q_x) + \cos(k_y \pm Q_y))]^2}$$

which is taken to be repulsive ($\lambda > 0$) and to have maxima at variable $Q_x, Q_y$ with peak widths characterized by $J_o$. The magnetic pairing scenario is a special case of this more general interaction with $Q_x = Q_y = \pi/a$. As expected from the Kohn Luttinger picture, if this interaction is substituted into Eq(1), a variety of anisotropic pairing states will arise. The various allowed symmetries are plotted in Figure 1 as a function of $Q_x, Q_y$. Here the electronic structure is taken to be that of YBCO, near optimal stoichometry where the Van Hove singularities (or flat band regions) are in close proximity to the Fermi surface.

An important conclusion of this study is that the largest fraction of phase space is associated with $d_{x^2-y^2}$ pairing. Thus, one may conclude that this symmetry should not be related to any particular wave vector structure. It appears to be a robust consequence of superconductivity driven by repulsive interactions. What stabilizes this $d_{x^2-y^2}$ pairing state over other candidate states? There are two important effects: (1) it is a state with a minimal number of sign changes in the gap function, (as compared to the eight lobe $s$-state ($A_{1g}$) also shown) and consequently yields higher $T_c$’s for most slowly varying interactions and (2) it is a state which takes maximal advantage of
the high density of states associated with the flat band regions or "Van Hove" effects. Moreover, these flat bands are observed experimentally in a variety of cuprates. It should be stressed that our early work has noted that correlation effects contribute in an important way to pin the flat bands near the Fermi energy, so that these effects should not be interpreted as simple (i.e., one electron) Van Hove singularities.

Despite these suggestive results, a more microscopic picture is clearly desirable. The most natural source for a repulsive interaction which may drive the superconductivity in the cuprates, is the direct Coulomb interaction. Moreover, it is essential to our work that we begin with the full long range Coulomb interaction, rather than the Hubbard model approximation. We have, therefore, generalized the Kohn Luttinger calculation based on the screened Coulomb interaction to the case of a two dimensional, tight binding lattice. Here we find two important effects play a role in our analysis: local field and Van Hove contributions. Local field effects lead to a matrix form for the dielectric constant, so that higher Brillouin zone contributions or Umklapp processes are included.

In Figure 2a we plot our results for the screened Coulomb interaction for LaSrCuO (at optimal stoichiometry) and, as a point of comparison, for three dimensional jellium. The results for the YBaCuO family are found to be similar. The effect of the flat band regions enters not only in the density
of states effects discussed in the context of the simple generic model in Figure 1, but also directly into the interaction itself. These large density of states regions cause a dip in the interaction associated with enhanced screening. This dip is then followed by a maximum, slightly above the \((\pi/a, \pi/a)\) point. Moreover these Van Hove effects are enhanced further through higher zone or Umklapp processes as shown in the inset. Finally, and most importantly, the superconducting instability associated with this wave vector structure is indeed, the \(d_{x^2-y^2}\) state.

In Figure 2b we plot the screened Coulomb interaction in co-ordinate space in the static limit. This figure shows the expected Friedel oscillations, which (in the Kohn Luttinger language) may be viewed as driving the superconductivity. The characteristic energy scale beyond which the Friedel oscillations become significantly altered, so that the d-wave pairing is no longer stable, is of the order of \(4t\) (where \(t\) is the nearest neighbor hopping). This cut-off thus represents a sizeable fraction of the plasma frequency.

What about the characteristic size of \(T_c\)? We are in the process of introducing corrections to the mean field equation which include phase fluctuation effects and which will enable us to compute \(T_c\) more reliably. These phase fluctuation effects are manifested in "pseudo-gap" behavior away from optimal stoichiometry. It is only when such a scheme is in hand that we can with some confidence make further progress on the pairing mechanism.

In summary, this paper has demonstrated the generality of the \(d_{x^2-y^2}\) pairing symmetry and has suggested an alternate route to d-wave pairing via the long range Coulomb interaction. Whether this is all or only a component of the pairing is too soon to say, but it is clear that direct Coulombic effects will act in concert with any other underlying d-wave pairing mechanism.

This work is supported by the National Science Foundation (DMR 91-20000) through the Science and Technology Center for Superconductivity.

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