On a theoretical model for d-wave to mixed s- and d-wave transition in cuprate superconductors

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Abstract. A $U(\beta)$ model proposed by Iachello for superconductivity in cuprate materials is analyzed. The model consists of $s$ and $d$ pairs (approximated as bosons) in a two-dimensional Fermi system with a surface. The transition occurs between a phase in which the system is a condensate of one of the bosons, and a phase which is a mixture of two types of bosons. In the current work we have investigated the validity of the Bogoliubov approximation, and we used a reduced Hamiltonian to determine a phase diagram, the symmetry of the phases and the temperature dependence of the heat capacity.

For more than a decade there has been a debate regarding the nature of the symmetry of the macroscopic wavefunction for the copper oxide superconductors. According to Müller bulk sensitive experiments support substantial $s$ symmetry, while surface sensitive experiments yield $d$ symmetry for the macroscopic wave function. Müller proposed \cite{1} that a reconciliation of the conflicting experiments was possible if the superconducting wavefunction were a sum of two components, namely, one of $s$ symmetry and one of $d$ symmetry, and var-

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ied as a function of the distance from the surface.

Following that work by Müller, a theoretical framework for cuprate superconductors was proposed by Iachello [2], based on the analogy with atomic nuclei. In the present work we report our analysis of phase transitions based on Iachello’s model. Also we have investigated temperature dependence of the heat capacity. We propose a macroscopic wavefunction for realizing space dependence.

In Eq[1] we give Iachello’s Hamiltonian for $2N$ spin $\frac{1}{2}$ fermions on a plane. This is a boson Hamiltonian [3], which consists of three types of bosons $s, d_+$ and $d_-$.

\begin{equation}
H = \varepsilon_s \hat{s}^\dagger \hat{s} + \varepsilon_d \hat{d}^\dagger \hat{d} + u_0 \hat{s}^\dagger \hat{s} \hat{s} + u_2 \hat{d}^\dagger \hat{d} \hat{s} + u_3 \hat{d}^\dagger \hat{s} \hat{d} + v_0 \hat{d}^\dagger \hat{d} + v_2 \hat{d}^\dagger \hat{s} \hat{d} + \hat{s} \hat{d} + \hat{d} \hat{s} + v_2 \hat{d}^\dagger \hat{s} \hat{d} + \hat{s} \hat{d} \hat{s} \hat{d}
\end{equation}

Introducing the operators [2]

\begin{align}
\hat{n}_s &= \hat{s}^\dagger \hat{s} \\
\hat{n}_d &= \hat{d}^\dagger \hat{d} \\
\hat{n}_s &= \hat{n}_d \hat{n}_d + \hat{n}_d \\
\hat{l} &= \hat{n}_d + \hat{n}_d \\
\hat{N} &= \hat{n}_d + \hat{n}_d
\end{align}

the Hamiltonian can be rewritten as

\begin{equation}
H = \varepsilon_s \hat{n}_s + \varepsilon_d \hat{n}_d + u_0 \hat{n}_s \hat{n}_d + u_2 \hat{n}_d \hat{n}_d + u_3 \hat{n}_d \hat{n}_d + v_0 \hat{n}_d \hat{n}_s + v_2 \hat{n}_d \hat{n}_d + \hat{n}_d \hat{n}_d + \hat{n}_d \hat{n}_d
\end{equation}

Its algebraic structure is $U(3)$

\begin{align}
\hat{n}_s &= \hat{s}^\dagger \hat{s} \\
\hat{n}_d &= \hat{d}^\dagger \hat{d} \\
\hat{d}_s &= \hat{d}_s \hat{d}_s + \hat{d}_s \hat{d}_s \\
\hat{d}_d &= \hat{d}_d \hat{d}_d + \hat{d}_d \hat{d}_d \\
\hat{l} &= \hat{d}_s \hat{d}_s + \hat{d}_d \hat{d}_d \\
\hat{N} &= \hat{d}_s \hat{d}_s + \hat{d}_d \hat{d}_d
\end{align}

This algebra contains a subalgebra $SO(3)$ formed from the generators $\hat{T}_+, \hat{T}_-, \hat{l}$, and a Casimir operator defined as (note a factor of 2 difference from Ref. [2])

\begin{equation}
\hat{W}^2 = \hat{T}_+ \hat{T}_- + \hat{l}^2
\end{equation}
Following Iachello this Hamiltonian can be split into an $SO(3)$ symmetric part, which will contain $\hat{l}$ and $\hat{W}^2$ terms, and a $U(1)$ $U(2)$ symmetric part generated by $\hat{n}_s$ and $\hat{I}_s\hat{n}_d\hat{Q}$, respectively. When the Hamiltonian has $SO(3)$ symmetry the system is in phase II, which corresponds to a mixture of $s$- and $d$- bosons. When the Hamiltonian has $U(1)$ $U(2)$ symmetry the system is in phase I, which corresponds to either an $s$- boson condensate (phase Ia) or a $d$- boson condensate (phase Ib).

As shown in Ref. [2] an analytical solution could be obtained either for phase I or phase II, but in intermediate situations one could only obtain an approximate or a numerical solution. Since we have three kinds of bosons in the model and a macroscopic number of particles, we may use the Bogoliubov approximation [3]. This approximation consists of replacing in the Hamiltonian (1) the operators which create and annihilate bosons in the condensed state by a c-number and neglecting all terms higher than degree two in operators which annihilate and create bosons in other states. After this replacement the Hamiltonian becomes the bilinear form

\[
\begin{align*}
H_d &= H_0 + (\varepsilon_s + \nu_0 N_d + \mu) \hat{n}_s + \\
&+ \frac{1}{2} \nu_2 \frac{N_d^2}{l^2} \hat{s}^\dagger \hat{s} + \hat{s}^\dagger \hat{s} \\
H_0 &= (\varepsilon_d - \mu) N_d + \frac{1}{4} 2u_2 + u_2^0 N_d^2 + \frac{1}{4} 2u_2 + u_2^0 l^2
\end{align*}
\]

where $\hat{d}^\dagger \hat{d} \not\to N_d = N_+ + N_-$; $l = N_+ N_-$ and $\mu$ is a chemical potential. The chemical potential is determined as usual from the condition on the mean total number of particles. $N_d$ is determined by variation. To diagonalize the bilinear form (4) we introduce the squeezing transformation

\[
U_s = \exp \frac{\alpha}{2} \hat{s}^\dagger \hat{s}^2
\]

We compare the Bogoliubov approximation with the exact numerical solution in Fig 1. The right column of Fig 1 shows the occupancy of the $s$-bosons. We observe different regions of the parameter corresponding to different phases of the system. The left column shows
that the Bogoliubov approximation gives remarkably good results either when the system is in phase Ia or phase II: The failure of the Bogoliubov approximation in phase Ib is expected since the s-level is not macroscopically occupied in that phase. (Another Bogoliubov approximation based on macroscopic occupancy of only d-bosons could be constructed for phase Ib)

In order to investigate the transition between phase I and phase II the original Hamiltonian can be reduced to the form

$$H = \varepsilon \hat{n}_d \frac{v_2}{2} \hat{W}^2$$

(by setting $\varepsilon_s = v_0 = 2u_2 = 2u_2^0 = v_2; u_0 = 0$ and $\varepsilon = \varepsilon_d + \frac{1}{2}v_2$)

This Hamiltonian contains the essential features required to describe the transition between the phases. The system is in phase I for $v_2 = 0$ and it is in phase II for $\varepsilon = 0$: In the first case the system reduces to a simple two level system of $N$ non-interacting bosons, and in the second case we have pure pairing interaction. In order to have a quantitative measure of $s$-wave and $d$-wave symmetry we define two fractional weight operators

$$\hat{g}_d \frac{1}{N} \hat{n}_d \quad \hat{g}_s \frac{1}{N} \hat{n}_s;$$
and the fractional weight measures of a state $\Psi$:

$$S = \frac{1}{h} \langle \hat{g}_s \hat{g}_s \rangle$$ $D = \frac{1}{h} \langle \hat{g}_d \hat{g}_d \rangle$$

with the properties

$$D_0 = 1; \quad D_{N=2} = \frac{1}{2}; \quad D_N = 0$$

$$S_0 = 0; \quad S_{N=2} = \frac{1}{2}; \quad S_N = 1$$

where the subscripts $0; N$ and $N$ indicate $\Psi = \Psi; N \Psi; \frac{N}{2}; \frac{N}{2}; \frac{N}{2}; \Psi; 0 \Psi$ respectively.

For pure $s$-wave symmetry $S$ and $D$ yield one and zero, respectively, and vice-versa for pure $d$-wave symmetry. For mixed symmetries, $S$ and $D$ vary between zero and one.

A phase diagram of the system described by the reduced Hamiltonian may be obtained readily by calculating the $s$-wave or the $d$-wave symmetry measure in the exact ground state for different values of $v_2$ and $\varepsilon$.

As seen from Fig. the system has three distinct phases. When the system is in phase $I$ the number of $s$- and $d$- bosons is definite;
when it is in phase $II$ the number of $s$- and $d$-bosons is indefinite. The transition between the phases can be controlled by changing $\varepsilon$ or $v_2$:

The strength of the scattering interaction ($v_2$) could be controlled by the doping of the superconducting sample. It is known that doping affects electron-electron and electron-phonon scattering [5], therefore the desired scattering on the Fermi surface could be achieved by varying the doping of the sample (Meir Weger, private communication).

Having the exact numerical solution we can examine the thermodynamical properties of this model by calculating the free energy and the density matrix of the system at inverse temperature $\beta$

\[
Z = \text{Tr} e^{-\beta H} \quad F = \frac{1}{\beta} \ln Z \quad \hat{\rho} = \frac{1}{Z} e^{\beta H}
\]

We can then explore the behavior of the derivatives of the free energy with respect to the temperature. The first and the second derivatives of the free energy are shown to be continuous functions at the explored domain of parameters. However, there is a jump in the second derivative when the temperature scale is of the same order as the difference between the ground and first excited states (Fig 3).

This jump does not become a singularity point when the number of particles tends to infinity, since the width of the peak does not scale as $N^{\alpha}$, and therefore there is no second order phase transition at this point [6].

Although there is no second order phase transition, changing the temperature does produce a transition between phases having different symmetries. If the system is in phase $I$ at $T = 0$; we can calculate the mean ensemble $s$-wave and $d$-wave symmetry measures as a function of the temperature

\[
\bar{S} = \text{Tr} (\hat{g}_s \hat{\rho}) \quad \bar{D} = \text{Tr} (\hat{g}_d \hat{\rho})
\]

In Fig. 4 we present the temperature dependence of $\bar{S}$ and $\bar{D}$: We observe that both symmetry measures approach $\frac{1}{2}$ when the temperature is increased, which corresponds to phase $II$ of the system. If the system is initially in phase $II$, it would remain in this phase.
Figure 3. The entropy (solid line) and the specific heat of the system (dashed line) as a function of the temperature. For $T = 0$ the system is in phase $Ib$.

Figure 4. Mean symmetry measures as functions of the temperature. The solid line denotes the $s$-wave symmetry measure and the dashed line denotes the $d$-wave symmetry measure. For $T = 0$ the system is in phase $Ib$:

...for any temperature. It is tempting to propose the temperature as the control parameter for the transition, but some things should be kept in mind. First, the temperature scale of the transition may be higher than the critical temperature of the superconductor. This can only be known after the model is fit to experimental data and the values of the Hamiltonian parameters are obtained. Second, if we would like the temperature to be the control parameter of the transition, there must be a temperature gradient within the copper-oxide plane of the superconductor, so that the bulk of the superconductor will have higher temperature than its surface. This is not likely to happen since the superconductor is in thermal equilibrium and the typical surface depth is of the order of only several atomic layers.

To sum up, in this work we have used a theoretical model proposed by Iachello for a transition from $d$-wave to mixed $d$- and $s$-wave symmetry. A phase diagram of the model was obtained, which showed a distinct separation between the three phases. Doping of the superconducting sample and temperature were proposed as possible...
control parameters for the phases of the system.

Acknowledgements

We would like to thank Meir Weger for his considerable help. JLB thanks the Institute of Theoretical Physics of Technion for its support and hospitality. Also support from PSC-CUNY is acknowledged.

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