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Charged boson condensation in high-T_c superconductors

Xiao-Gang Wen* and Rui Kan
Joseph Henry Laboratories, Princeton University, Princeton, New Jersey 08544
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We explore the superconducting transition in the RVB (resonant valence bond) model, assuming that the superconductivity is due to a Bose-Einstein condensation of charged bosons in the RVB vacuum. It appears that the charged bosons behave like a weakly interacting $2+\epsilon$ dimensional boson gas and that the RVB superconductors exhibit many two-dimensional properties. Among others are a linear temperature dependence of the critical fields, which has already been observed in experiments, and a linear doping dependence of the transition temperature.

Among various theoretical explanations of the high-T_c superconductors, the resonant valence bond (RVB) model proposed by Anderson and co-workers[1,2] is quite successful and there is no known experimental data contradicting this theory.[3-5] In this paper we are going to explore a possible mechanism of superconductivity in the RVB vacuum, i.e., Bose-Einstein condensation of charged particles.[3,4] While pair breaking may play a role in many circumstances, it is worthwhile to explore the suggestion that Bose-Einstein condensation is dominant at least for low doping. There are three kinds of important excitations in the RVB vacuum, an unbonded spin (spinon), an empty site (hole), and a charged electron. It is a crucial property of the RVB vacuum that the spinons are neutral fermions and the holes are charged bosons.[3,4] In real RVB superconductors there is a net number of the holes, and the total number of the holes is conserved. Therefore, under certain conditions, the holes should be able to condense and give rise to the observed superconductivity of the high-T_c superconductor. In this paper, we calculate the transition temperature, the critical fields, and the specific heat of RVB superconductors. We also estimate the range of the critical region. We find that the holes exhibit many two-dimensional properties. Some of these properties have already been observed in experiments.[6,7]

In the RVB vacuum, the motion of the holes is constrained to Cu layers and the holes essentially behave like a two-dimensional boson gas. It is well known that a two-dimensional boson gas does not condense; therefore, interlayer couplings play an important role in the boson condensation. It is not known whether the interlayer couplings are due to single-hole hopping $\phi_i\phi_j^*$ or double-hole hopping $\phi_i^2\phi_j^{*2}$, where ϕ_i is the wave function of the holes in the ith Cu layer. But present RVB theory favors double hole hopping. In any case, the interlayer couplings are weak. This is because the wave functions of the valence electrons in different layers do not overlap. The interlayer hoping for valence electrons (and the holes) is extremely small. We expect that many properties of the superconducting state, including the properties discussed in this paper, do not depend on details of the interlayer couplings (although the structure of the order parameter and macroscopic quantum effects depend on whether the couplings are due to single-hole hopping or double-hole hopping.[5]) These properties depend on the couplings only through a parameter characterizing the coupling strength; therefore, they can be studied by assuming that the interlayer couplings are due to single-hole hopping. This is equivalent to giving the holes a large effective mass in the z direction (we choose the z axis to be perpendicular to the Cu layer). In addition to the assumption about interlayer couplings, we also assume that the interaction between the holes is weak, because of the strong screening effect of charged boson gas. The free-boson picture is at least qualitatively sufficient to describe the superconducting transition in the RVB vacuum. The two-body interaction between the holes is important only to generate a nonzero thermal critical field H_c and a jump of specific heat at the transition.

Because the holes are almost localized in the z direction, we expect that there is a large energy gap between different energy bands in the k_z direction. Therefore, only the first band is important. The single-particle energy spectrum may be written as

$$\varepsilon_{\mathbf{p}}=\frac{1}{2m}(p_x^2+p_y^2)+\frac{1}{Md^2}[1-\cos(p_zd)] \ , \qquad (1)$$

where d is the distance between Cu layers. We would like to emphasize that under temperatures of interest, the bandwidth in the k_z direction $M^{-1}d^{-2}\ll k_BT$. (Because there is no valence bond between layers, the hole cannot hop between layers itself in the RVB theory, it has to hop together with a spinon, and, therefore, the effective mass M is very large.) The spectrum in (1) describes quasi-two-dimensional particles. To study Bose-Einstein condensation of such a quasi-two-dimensional gas, let us first ignore the interaction between the holes. The thermopotential for free bosons with energy spectrum (1) can be written as

$$\Omega_0=-V\frac{k_BT}{\lambda^2d}\sum_{l=1}^{\infty}l^{-2}I\left(\frac{l}{k_BTMd^2}\right)e^{\mu l/k_BT} \ , \qquad (2)$$

where $\lambda=(2\pi/mk_BT)^{1/2}$ and

$$I(s)=\int_0^1\exp\{-s[1-\cos(2\pi t)]\}dt \ .$$

Noticing that $I(s\ll 1)\simeq 1$ and $I(s\gg 1)\simeq(2\pi s)^{-1/2}$, we may express the density of the holes in excited states as

$$n-n_s=\lambda^{-2}d^{-1}\sum_{l=1}^{\infty}l^{-1}I\left[\frac{l}{k_BTMd^2}\right]e^{\mu l/k_BT}$$
$$=-\lambda^{-2}d^{-1}\ln\left[\frac{t}{\nu(t)}\right],\ \text{for}\ \mu=0\ , \quad (3)$$

where $n=N/V$ is the density of the holes, n_s is the density of the condensed holes, $t=1/k_BTMd^2$, and $\nu(t)$ is a function of order $O(1)$ which approaches a non-zero constant as $t\rightarrow 0$. From (3) we see that there is boson condensation below a certain transition temperature T_c. Assuming t is small, we find that

$$k_BT_c=\frac{2\pi nd}{m\ln(k_BT_cM\nu d^2)}\ . \quad (4)$$

Note that T_c is very insensitive to the effective mass in the z direction when nMd^3/m is large. With a reasonable choice of M, $\ln(k_BT_cMd^2\nu)\sim 10$. In the large nMd^3/m limit, the density of the condensed holes reads

$$n_s=n-\frac{1}{\lambda^2d}\ln(k_BTMd^2\nu)\simeq n\frac{T_c-T}{T_c}\ . \quad (5)$$

The free energy of the noninteracting holes $F_0=\Omega_0+\mu N$ can be obtained by solving the chemical potential μ from (3).

The free energy obtained above is very complicated; for later convenience we would like to show that the above free energy can be approximated by the free energy of a $2+\epsilon$ dimensional free boson gas. By definition, such a $2+\epsilon$ dimensional boson gas is described by the following thermopotential:

$$\Omega_\epsilon=-\frac{Vk_BT}{\lambda^2d}\sum_{l=1}^{\infty}l^{-2-1/2\epsilon}e^{\mu l/k_BT}$$
$$=-\frac{Vk_BT}{\lambda^2d}g_{2+\epsilon/2}(e^{\mu/k_BT})\ , \quad (6)$$

where $g_a(s)=\sum_{l=1}^{\infty}l^{-a}s^l$. The chemical potential is determined by

$$n-n_s=\lambda^{-2}d^{-1}g_{1+\epsilon/2}(e^{\mu/k_BT})\ . \quad (7)$$

The $2+\epsilon$ dimensional free boson gas undergoes a condensation at a temperature

$$k_BT_c=\frac{2\pi nd}{mg_{1+\epsilon/2}(1)}\ . \quad (8)$$

We see that (8) will agree with (4) if we set

$$g_{1+\epsilon/2}(1)=\ln(k_BT_cMd^2\nu)\ , \quad (9)$$

which is equivalent to

$$\epsilon=2\left[\ln\left[\frac{nMd^3}{m}\right]\right]^{-1}\ , \quad (10)$$

for small ϵ. Above the transition temperature, one can easily see that $\Omega_0\simeq\Omega_\epsilon$ and $\partial\Omega_0/\partial\mu\simeq\partial\Omega_\epsilon/\partial\mu$, for $-\mu/k_BT\gg\epsilon$ and $\epsilon\ll 1$. At the transition temperature $\partial\Omega_0/\partial\mu=\partial\Omega_\epsilon/\partial\mu$ by (9). Below the transition temperature, the thermopotentials for both systems are approximately equal to a constant, and so are the free energies

$$F_0\simeq F_\epsilon\simeq-\frac{k_BTV}{\lambda^2d}g_{2+\epsilon/2}(1)\ . \quad (11)$$

So the free energy of the noninteracting holes and the free energy of $2+\epsilon$ dimensional free boson gas are approximately the same for all temperatures, if the effective mass M is large and ϵ is small.

With the help of the above approximation, we may write the free energy of the holes as

$$\frac{F_\epsilon}{V}=\begin{cases}-\dfrac{k_BT}{\lambda^2d}g_{2+\epsilon/2}(e^{\mu/k_BT})+\mu n, & \text{if}\ T>T_c\ ;\\ -\dfrac{k_BT}{\lambda^2d}g_{2+\epsilon/2}(1), & \text{if}\ T<T_c\ ;\end{cases} \quad (12)$$

where μ is determined by (7). From (12) we may easily calculate the specific heat of the holes and find that $\Delta c=0$ at the transition point. This implies that $(dH_c/dT)_{T_c}=0$ for the noninteracting holes. It is well known that the interaction between bosons can generate nonzero Δc, therefore, the nonzero dH_c/dT observed in experiments is totally due to the interaction between the holes. Including a two-body interaction characterized by scattering length a, the total energy of the holes for low-lying states reads[8]

$$E=\sum_{\mathbf{p}}n_{\mathbf{p}}\varepsilon_{\mathbf{p}}+\frac{4\pi a}{mV}\left[N^2-\tfrac{1}{2}N-\tfrac{1}{2}\sum_{\mathbf{p}}n_{\mathbf{p}}^2\right]\ , \quad (13)$$

where $\varepsilon_{\mathbf{p}}$ is the single-particle kinetic energy and $n_{\mathbf{p}}$ is the occupation number of the $\mathbf{p}$ state. Equation (13) is valid in low-temperature and low-density limits, i.e.,

$$\frac{a}{d}\ll 1,\ a\left[\frac{k_BTm}{2\pi}\right]^{1/2}\ll 1,\ an^{1/3}\ll 1\ . \quad (14)$$

We will find later that $a\sim 0.05$ Å and $m\sim 1.5m_e$, hence, the above condition is indeed valid. Noticing that of all the $n_{\mathbf{p}}$'s none except $n_{\mathbf{p}=0}$ is expected to be macroscopically large, thus, we may write

$$E=\sum_{\mathbf{p}}n_{\mathbf{p}}\varepsilon_{\mathbf{p}}+\frac{4\pi aV}{m}\left[n^2-\frac{1}{2}n_s^2\right]\ . \quad (15)$$

Observing that the total energy is shifted only by a constant, the free energy for the interacting holes may be written as

$$\frac{F}{V}=-\frac{k_BT}{\lambda^2d}g_{2+\epsilon/2}(e^{\mu/k_BT})+\mu(n-n_s)+\frac{4\pi a}{m}\left[n^2-\frac{1}{2}n_s^2\right]=\begin{cases}-\dfrac{k_BT}{\lambda^2d}g_{2+\epsilon/2}(e^{\mu/k_BT})+\mu n+\dfrac{4\pi a}{m}n^2, & \text{if}\ T>T_c\\ \dfrac{4\pi a}{m}\left[n_s^2/2-n\dfrac{T_c-T}{T_c}n_s+n^2\right]-\dfrac{k_BT}{\lambda^2d}g_{2+\epsilon/2}(1), & \text{if}\ T<T_c,\end{cases} \quad (16)$$

where μ is determined by (7) and n_s by minimizing F. It is not hard to see that the transition temperature and density of the condensed holes are the same as before [see (8) and (5)]. The specific heat may be easily calculated as

$$c = k\left[\frac{m}{\pi d} g_{2+\epsilon/2}(1) + \frac{4\pi a n^2}{m(k_B T_c)^2}\right] k_B T \ , \tag{17}$$

for $T < T_c$, and is the same as that of the noninteracting holes for $T > T_c$. The jump of the specific heat at the transition temperature is

$$\Delta c = k \frac{4\pi a n^2}{m k_B T_c} \ . \tag{18}$$

In presence of magnetic field, the system has two possible states, a normal state ($n_s = 0$) and a superconducting state ($n_s \neq 0$). In the normal state, the magnetic field penetrates the system. There is no condensation because of the appearance of Landau levels, hence none of the $n_{\mathbf{p}}$'s in (18) is macroscopically large. Noticing that the magnetic susceptibility of the system is always small, the free energy of the normal state can be written as

$$F_N(H \neq 0) = F_\epsilon + \frac{4\pi a V n^2}{n} \ . \tag{19}$$

Comparing with the free energy for superconducting state $F_S = F + H^2 V/8\pi$, we obtain the thermal critical field

$$H_c = 4\pi n \left[\frac{a}{m}\right]^{1/2} \frac{T_c - T}{T_c} \ . \tag{20}$$

From (5), we obtain the temperature dependence of the penetration length of the superconductor

$$\lambda_{p\perp}^2(T) = \frac{mc^2}{4\pi e^2 n} \frac{T_c}{T_c - T} \ , \tag{21}$$

as well as the lower critical field

$$\begin{aligned} H_{c1\perp} &= \frac{\Phi_0}{2\pi\lambda_p^2(0)} \ln\left[\kappa \frac{T_c - T}{T_c}\right] \\ &= \frac{e g_{1+\epsilon/2}(1)}{cd} k_B (T_c - T) \ln\kappa \ . \end{aligned} \tag{22}$$

Since we have used the mass of the holes in (21), the above two formulas are only valid when magnetic field is perpendicular to the Cu layers. We will discuss other situations later.

In order to write down the Ginsberg-Landau (GL) equation, we choose the order parameter to be the wave function of the condensed holes ϕ_i, where i refers to the ith Cu layer. Allowing a spatial dependence of the order parameter and including kinetic terms, the total free energy now reads

$$F = F_N + \sum_i \int dx\, dy \left[4\pi \frac{ad}{m}\left[n_s^2/2 - n\frac{T_c - T}{T_c} n_s\right] + \frac{1}{2m}(|\partial_x \phi_i|^2 + |\partial_y \phi_i|^2) - \frac{1}{2Md^2}|\phi_{i+1} - \phi_i|^2\right] \ , \tag{23}$$

where $n_s = |\phi_i|^2/d$. The above free energy and the derived GL equation have been proposed to describe weakly coupled superconducting layers and have been studied by many people.[9] From the free energy (23) one may easily obtain the penetration and correlation lengths in any directions, e.g.,

$$\begin{aligned} \lambda_{p\perp}^2(T) &= \frac{mc^2}{4\pi e^2 n} \frac{T_c}{T_c - T} \ , \\ \lambda_{p\parallel}^2(T) &= \frac{Mc^2}{4\pi e^2 n} \frac{T_c}{T_c - T} \ , \\ \xi_{xy}^2 &= (8\pi n a)^{-1} \left|\frac{T_c}{T_c - T}\right| \ , \\ \xi_z^2 &= (8\pi n a)^{-1} \frac{m}{M} \left|\frac{T_c}{T_c - T}\right| \ , \end{aligned} \tag{24}$$

where ξ_{xy} is the correlation length in the x-y plane and ξ_z is in the z direction. The ratios of the penetration and correlation lengths are

$$\begin{aligned} \kappa_\perp &\equiv \frac{\lambda_{P\perp}}{\xi_{xy}} = \left[\frac{2amc}{\alpha}\right]^{1/2} \ , \\ \kappa_\parallel &= \frac{\lambda_{P\parallel}}{\xi_z} = \frac{M}{m} \kappa_\perp \ , \end{aligned} \tag{25}$$

where α is the fine-structure constant. The upper critical field perpendicular to the Cu layer is given by

$$H_{c2\perp}(T) = \sqrt{2}\kappa_\perp H_c(T) \ . \tag{26}$$

Since $\xi_z \lesssim d$ for almost all temperatures below T_c in this model, the lower and upper critical fields parallel to Cu layers are given by[9]

$$\begin{aligned} H_{c1\parallel} &= \left[\frac{m}{M}\right]^{1/2} \frac{\Phi_0}{2\pi\lambda_{P\perp}^2} \left[\frac{2\lambda_{P\perp}}{\pi^2 d}\right]^{1/2} \\ &\sim 0 \\ H_{c2\parallel} &= \left[\frac{m}{M}\right]^{1/2} \left[1 - \frac{d^2}{2\xi_z^2}\right]^{-1} \frac{\Phi_0}{2\pi d^2} \\ &= \infty \ \text{for } \xi_z < d/\sqrt{2} \ . \end{aligned} \tag{27}$$

Since $M \gg m$, (27) implies that $H_{c2\parallel} = \infty$ for almost all temperatures below T_c. The results in (27) are obtained from a mean-field theory; however, we expect that the fluctuations are important in calculating $H_{c2\parallel}$. The finite upper critical field observed in experiment is probably a critical phenomenon. At low temperatures, $H_{c2\parallel}$ may be limited by other physical mechanisms, for example, the Pauli limit.

In the above calculations, the GL equation is treated as a mean-field theory. The mean-field approximation is incorrect near the transition temperature where the effects of fluctuations are large. To estimate the importance of the fluctuation, we may compare the specific heat $c_{\rm fluct}$ arising from the fluctuations with the jump of the specific heat Δc obtained from the mean-field theory. Using the Gaussian approximation, we obtain

$$\frac{c_{\rm fluct}}{\Delta c}=\zeta\frac{T_c}{T_c-T}\ , \qquad (28)$$

near the transition, where

$$\zeta\simeq\frac{\epsilon}{4}\left(1+\frac{1}{2\pi nad^2}\frac{m}{M}\frac{T_c}{T_c-T}\right)^{-1/2}$$
$$\simeq\frac{\epsilon}{4} \qquad (29)$$

The fluctuations are important when $c_{\rm fluct}\gtrsim\Delta_c$, or $|T-T_c|\lesssim\zeta T_c$. Since ϵ is small for RVB superconductors, our previous results are valid for almost all temperatures except for temperatures in the critical region $|T-T_c|\lesssim\zeta T_c$. The critical region shrinks to zero as $a\to 0$. This is expected since our results are exact for free bosons. We should emphasize that the critical region for RVB superconductors, which is of order of several tenths of a degree wide, is huge compared to that of BCS superconductors, which can be as narrow as $10^{-15}T_c$. The critical phenomena for RVB superconductors can be easily observed and probably have already been observed in Refs. 10 and 7. In Ref. 10, $H_{c2\perp}$ is found to behave as $(T_c-T)^{3/2}$ near T_c.

Now let us compare our results with experiments. Choosing proper values for ϵ, m, and a to fit the experimental data, we obtain the following for La-Sr-Cu-O samples with 0.15 doping[6,11]

$$\epsilon^{-1}=37,\ m=1.4m_e,\ a=0.05\ \text{Å},\ T_c=40\ \text{K}\ ,$$
$$\kappa_\perp=70,\ H_c=4500\ \text{G},\ H_{c2\perp}=44\ \text{T},\ H_{c1\perp}=200\ \text{G}\ , \qquad (30)$$

where we have assumed that some of the holes are localized and effective doping is 0.1. For Y-Ba-Cu-O samples with 0.4 holes per unit cell, we obtain[12]

$$\epsilon^{-1}=31,\ m=1.6m_e,\ a=0.023\ \text{Å},\ T_c=90\ \text{K}\ ,$$
$$\kappa_\perp=50,\ H_c=1.3\ \text{T},\ H_{c2\perp}=88\ \text{T},\ H_{c1\perp}=700\ \text{G}\ . \qquad (31)$$

We find that the effective masses of the holes are about the same for the two samples. This is a nontrivial check of our theory. Because the Cu layers are almost identical for the two samples and interlayer interactions are weak, it is expected that the effective masses of the holes are the same. We would like to point out that the results in (30) and (31) are obtained by comparing with the available experimental data on polycrystal samples (except $H_{c2\perp}$ for Y-Ba-Cu-O samples). Thus, the values that we obtain for ϵ, m, and a are not quite reliable. The strongest support of our theory comes from an experiment by Batlogg *et al.*[6] They find a linear temperature dependence of H_{c1} from 5 K to $T_c\sim 40$ K, with the slopes being independent of doping concentration. This agrees with our results in (22). Such linear temperature dependence is also observed in H_{c2} by Uchida *et al.*[7] Our theory also predicts a linear dependence of transition temperature on concentration of the holes. This agrees with a experiment by Shafer *et al.*[13] But their results are not accurate enough to exclude other possibilities, e.g., $T_c\propto n^{2/3}$ arising from three-dimensional Bose-Einstein condensation.

From the above comparisons, we find that the properties of the superconducting state of high-T_c superconductors can be consistently described by a weakly interacting $2+\epsilon$ dimensional charged boson gas. We believe that such a weak-interaction picture is correct for the holes in the RVB vacuum, at least for low doping. Experimental measurements of thermopower[14] also support such a picture.[15]

We would like to remark that the boson model discussed in this paper may also apply to the theories of superconductivity with very tide binding Cooper pairs, i.e., the size of the Cooper pairs is much smaller than the mean distance between the pairs. In this case, the bosons responsible for superconductivity carrying charge $2e$ (instead of e). We may still obtain an equally good fit to the experimental data. In RVB model, such tide binding pairs may arise from the RVB bonds.[3,4]

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*Present address: Institute for Theoretical Physics, University of California, Santa Barbara, Santa Barbara, CA 93106.

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