Condensation of Hard-Core Pairs on a Lattice: A Model of the Superconducting State in Cuprates

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Using the Monte Carlo technique we study the dependence of transition temperature, penetration depth and specific heat singularity on the pair concentration in the Bose Hubbard model. We observe remarkable agreement with the corresponding properties of cuprates. This points uniquely to Bose condensation of hard-core pairs on a lattice as the mechanism that drives the transition.

There is strong evidence that high-T_c-superconductors exhibit pronounced thermal fluctuation effects. In the Meissner phase, measurements of various properties, including the magnetic penetration depth and specific heat, clearly revealed that the fluctuations of the order parameter are essentially those of an uncharged superfluid or three dimensional (3D)-xy model. Indeed, remarkable consistency with the 3D-xy-critical point exponents and the universal relations between critical amplitudes and T_c has been established [1,2]. Moreover, it has been shown that these universal relations, supplemented by the empirical phase diagram (doping dependence of T_c), imply a doping-dependent effective pair mass and, in agreement with recent kinetic inductance [3] and μSR measurements [2], unconventional behavior of the penetration depth in the overdoped regime. The evidence for uncharged superfluid or 3D-xy behavior has been completed in terms of the asymptotic low-temperature dependence of the magnetic penetration depth, because the sound wave contribution of an uncharged superfluid accounts well for the experimental data [4]. This evidence for 3D-xy behavior, implying rather tightly bound and interacting pairs – even above T_c, together with the doping dependence of the effective pair mass points uniquely to Bose condensation of hard and interacting pairs on a lattice as the mechanism that drives the phase transition.

To substantiate this expectation we studied a model of hard pairs on a lattice by means of the Quantum Monte Carlo (QMC) and Monte Carlo (MC) technique. The organization of the paper is as follows: Firstly we sketch the model and define the quantities of particular interest. Secondly we present QMC results for the dependence of superfluid number density and T_c on pair concentration, and discuss their relation to the doping dependence of T_c and penetration depth in cuprate superconductors.

We consider the bosonic 3D Hubbard model describing hard pairs on a lattice [5]:

$$\mathcal{H} = -\sum_{<i,j>} t_{ij} b_i^\dagger b_j + U \sum_{<i,j>} n_i n_j \quad . \tag{1}$$

The sums extend over nearest-neighbors; $n_i = b_i^\dagger b_i$ denotes the number operator, $t_{ij} = t$ the hopping matrix element and U the strength of the repulsive nearest neighbor interaction. The quantities b and $b^\dagger$ are hard-core boson operators, because

$$[b_i, b_{j\neq i}^\dagger] = 0, \quad \{b_i, b_i^\dagger\} = 1, \quad [b_i, b_j] = 0, \quad [b_i^\dagger, b_j^\dagger] = 0. \tag{2}$$

This model undergoes a phase transition from the normal to the superfluid state. Using a wordline QMC technique and checkerboard decomposition with the Suzuki-Trotter formula [6,7], we calculated the specific heat for various pair concentrations (fillings) as a function of temperature. Using finite size scaling and system sizes from $4\times4\times4$ to $6\times6\times6$, we estimated T_c from the specific heat peak. Our estimates are depicted in Fig. 1 in terms of the normalized transition temperature, $\bar{T}_c = T_c/T_c^m$, versus pair concentration per site, ρ, where $0 \leq \rho \leq 1$. T_c^m is the transition temperature for $\rho = 0.5$, which happens to be the maximum T_c. For $\rho = 1$ all lattice sites are occupied by one pair. The diamonds denote the QMC estimates for $U = t$. This term describes an additional short-ranged repulsive interaction. In the limit $\rho \to 0$ and, due to particle hole symmetry, also for $\rho \to 1$ the system reduces to a dilute Bose gas, where $T_c \propto \rho^{2/3}$ and $T_c \propto (1-\rho)^{2/3}$ [5]. Around half filling, however, our estimates are better described by

$$\bar{T}_c = (4\rho(1-\rho))^{\frac{1}{3}} \tag{3}$$

corresponding to the solid curve in Fig. 1. Closely analogous results have been obtained for the case $U = 0$ (for $U > t$ the phase diagram will also contain charge-density-wave phases [5]). The generic behavior, namely that T_c increases with increasing pair concentration ρ, saturates at half filling, decreases as ρ is further increased, and exhibits particle hole symmetry, is remarkably close to the doping dependence of T_c in the cuprate superconductors [8,9]. In the present case, the decrease of T_c as the limit $\rho \to 1$ is approached, is easily understood, because for $\rho = 1$ all sites are occupied, the pairs become immobile and superfluidity is suppressed.

In this model the pair interaction is supposed to be heavily screened so that the Coulomb interaction becomes short-ranged. Nevertheless the charge 2e of the pairs will still lead to electrodynamic effects. In particular the London penetration depth λ can be expressed in terms of the helicity modulus Υ [10], which can be calculated with the QMC technique. The relation reads [11]

$$\frac{1}{\lambda^2} = \frac{16\pi^3}{\Phi_0^2}\Upsilon = \frac{16\pi n_s e^2}{Mc^2} \quad , \tag{4}$$

where Φ_0 is the fluxquantum. The latter equality relates the helicity modulus to the phenomenological London expression, where n_s is the superfluid number density and M the effective Ginzburg-Landau pair mass. From hydrodynamic considerations [15], we expect n_s to equal the number of pairs at zero temperature, so that $n_s(0) = n = \rho/V$, where V is the volume of the unit cell. We calculated the zero temperature helicity modulus and its dependence on the pair concentration. The results are shown in fig. 2 in terms of the concentration of superfluid pairs per site Υ versus pair concentration ρ. The solid curve corresponds to the simple relation [5]

$$\bar{\Upsilon}(0) = \rho(1-\rho), \qquad \bar{\Upsilon}(0) = \frac{a\Upsilon}{t} \quad , \tag{5}$$

where a denotes the lattice constant. This relation satisfies particle hole symmetry and interpolates correctly between the limits where superfluidity disappears. Here the dilute Bose gas behavior, $\bar{\Upsilon}(0) = \rho$ ($\rho \to 0$) and $\bar{\Upsilon}(0) = 1-\rho$ ($\rho \to 1$), applies. The discrepancies between the solid line and the calculated data can be attributed to finite size effects, the use of a finite number of Trotter slices and quantum fluctuations that are not properly taken into account by (5). Indeed, there are discrepancies from the dilute Bose gas behavior in the limits $\rho \to 0$ and $\rho \to 1$. In this model, the disappearance of superfluidity for $\rho \to 1$ is readily understood in terms of the effective pair mass M, which tends to infinity because all sites become occupied and hence the pairs are no longer mobile. This behavior leads to a rather unexpected ρ-dependence of the zero temperature value of the penetration depth, namely,

$$\lambda^{-2}(0) \propto \frac{\rho}{M} \propto \bar{\Upsilon}(0) = \rho(1-\rho) \quad . \tag{6}$$

It implies that the effective pair mass, M, depends on ρ, and in particular because $M \propto 1/(1-\rho)$, that it tends to infinity as ρ approaches 1. Thus, the vanishing transition temperature for $\rho = 1$ has been traced back to the divergence of the pair mass. Moreover, the penetration depth is seen to adopt its minimum value for $\rho = \frac{1}{2}$ and to increase as ρ approaches 0 or 1. Such behavior has recently been observed in the kinetic inductance measurements on $La_{2-x}Sr_xCuO_4$ [3]; in this experiment the doping dependence of the penetration depth has been studied in both the underdoped and overdoped regime.

To substantiate the analogy between superfluidity of hard pairs on a lattice and superconductivity in the cuprates, we turn to the specific heat anomaly and the universal properties of the 3D-xy-critical point. Indeed the phase transition in the hard pair model belongs to the 3D-xy-universality class. In this case T_c and the critical amplitudes of specific heat ($A^{\pm}$) and penetration depth (λ_0) are not independent of one another, but related by the universal relation [1,2]

$$(k_B T_c)^3 A^- = \left(\frac{\Phi_0}{16\pi^3}\right)^3 \frac{R_\varphi^3}{\lambda_0^6} \quad , \tag{7}$$

where $R_\varphi \approx 0.8$. The critical amplitudes are defined by the asymptotic behavior $\lambda = \lambda_0 t^{\nu}$ and $C = (A^{\pm}/\alpha)t^{-\alpha} + B^{\pm}$, where $t = |1-(T/T_c)|$ and $\alpha \approx 0, \nu \approx \frac{2}{3}$ and $A^+ \approx A^-$ for the 3D-xy-critical point. The universal relation (7) holds along the critical line $T_c = T_c(\rho)$ shown in Fig. 1, with the exception of the end points, $T_c = 0$ at $\rho = 0$ and $\rho = 1$. These end points correspond to 3D quantum xy critical points or, equivalently, to 3+1=4D classical xy critical points [12], where the mean field treatment becomes exact up to logarithmic corrections, and $A^{\pm}$ vanishes. Thus, $A^{\pm}$ is expected to adopt its maximum value for $\rho = \frac{1}{2}$ and to decrease as ρ tends to 0 or 1. In the critical region (close to T_c) classical thermal fluctuations dominate. For this reason we performed a classical MC study [13] of the specific heat by considering system sizes up to $16 \times 16 \times 16$. Invoking a finite size scaling analysis, we estimated the ρ-dependence of the critical amplitude $A^+ \approx A^-$. The results are shown in fig. 3 in terms of $\bar{A} = A/A\left(\rho = \frac{1}{2}\right)$ versus $\bar{T}_c = T_c/T_c\left(\rho = \frac{1}{2}\right)$. As expected, $\bar{A}$ is seen to decrease as ρ tends to 0 or 1. The solid line corresponds to

$$\bar{A} = \bar{T}_c^6 \quad , \tag{8}$$

which fits the data reasonably well. Analogous behavior has been found in the doping dependence of the specific heat singularity in $YBa_2Cu_3O_{7-\delta}$ [14]. Combining Eqs. (7) and (8) we find

$$\bar{T}_c \propto \left(\frac{1}{\bar{\lambda}_0^2}\right)^{\frac{1}{3}} \approx \left(\frac{1}{\bar{\lambda}^2(0)}\right)^{\frac{1}{3}} \quad , \tag{9}$$

where $\bar{\lambda}_0 = \lambda_0(\rho)/\lambda_0\left(\rho = \frac{1}{2}\right)$ and $\bar{\lambda}(0) = \lambda(T=0,\rho)/\lambda_0\left(T=0, \rho = \frac{1}{2}\right)$. In the last expression of Eq. (9) we assumed that $\bar{\lambda}_0$ and $\bar{\lambda}(0)$ exhibit nearly the same ρ-dependence. This expectation is nicely confirmed by combining Eqs. (6) and (9), which again yields (3). Accordingly, we provided a consistent picture of the ρ-dependence of the transition temperature T_c, the amplitude of the specific heat singularity A as well as of the penetration depth amplitude λ_0 and its zero temperature counterpart $\lambda(0)$. The decrease of T_c and the increase of penetration depth λ in the limit $\rho \to 1$ have been traced back to the ρ-dependence of the effective pair mass, which tends to infinity for $\rho \to 1$.

Remarkably enough, these essential features are fully consistent with those observed in cuprate superconductors. As a final illustration of this close analogy, we plotted in fig. 4 the μSR data [1,2] in terms of $\bar{T}_c$ versus $\bar{\lambda}(0)^{-2}$. With the approximate formulae from the QMC this gives

$$T_c \propto \left(\frac{1}{\lambda(0)}\right)^{\frac{1}{3}} \quad . \tag{10}$$

The experimental points of overdoped $Tl_2Ba_2CuO_{6+\delta}$ and $Ca_{1-x}Y_xSr_2Tl_{0.5}Pb_{0.5}Cu_2O_7$ confirm the essential implication of equation (10), namely, reversed evolution of underdoped (arrow up) and overdoped (arrow down) systems. The dashed lines, resembling the outline of a fly's wing, are a guide to the eye and illustrate the effect of breaking particle-hole symmetry. Indeed, the experimental points of overdoped $Tl_2Ba_2CuO_{6+\delta}$ and $Ca_{1-x}Y_xSr_2Tl_{0.5}Pb_{0.5}Cu_2O_7$ are close to the outline of the lower part of the wing, while the remaining data, referring to under- and mildly overdoped materials, are close to the upper part. The upper branch of the fly's wing corresponds to $T_c \propto (1/\lambda(0))^{2/3}$, which should hold in the dilute limit.

To summarize, the revealed analogy between hard pairs on a lattice and cuprate superconductors points uniquely to Bose condensation of hard pairs on a lattice as the mechanism that drives the phase transition.

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FIG. 1. The normalized transition temperature, $\bar{T}_c = T_c/T_c^{\mathrm{m}}$, vs. pair concentration per site obtained from QMC. The solid line corresponds to eq. (3). The dots are data extrapolated to the thermodynamic limit.

FIG. 2. The zero temperature helicity modulus, $\bar{\Upsilon}$, vs. pair concentration per site, ρ. The solid line corresponds to eq. (6). The diamonds are the QMC data for a $4 \times 4 \times 4$ system with 24 Trotter slices. The bars indicate the error arising from the extrapolation of finite temperature results to zero temperature.

FIG. 3. Normalized heat capacity critical amplitude, $\bar{A} = A/A^{\mathrm{m}}$ vs. the normalized transition temperature, $\bar{T}_c$. The solid line shows a fit to $\bar{A} \propto \bar{T}_c^{\,6}$, and the diamonds are the MC estimates.

FIG. 4. The normalized transition temperature, $\bar{T}_c$, versus $\bar{\sigma}(0) = \lambda(0)^{-2}/\lambda^m(0)^{-2}$. The solid line corresponds to Eq. (10), and the arrows denote the underdoped (up, $0 \leq \rho \leq \frac{1}{2}$) and overdoped (down, $\frac{1}{2} \leq \rho 1$) regimes. The dashed lines are a guide to the eye and sketch the effect of breaking the particle-hole symmetry, with the upper branch given by $(1/\lambda(0))^{2/3}$. Data taken from [1] and [2]:
$\boxdot$: $Tl_2Ba_2Ca_2Cu_3O_{10}$, $Tl_{0.5}Pb_{0.5}Sr_2Ca_2Cu_3O_9$, $Bi_{2-x}Pb_xSr_2Ca_2Cu_3O_{16}$, $\diamond$: $Y_{1-x}Pr_xBa_2Cu_3O_{6.97}$, $\triangle$: $YBa_2Cu_3O_x$, $\bigtriangledown$: $La_{2-x}Sr_xCuO_4$, $\star$: $Bi_2Sr_2Ca_{1-x}Y_xCu_2O_{8+\delta}$, $\odot$: $Tl_2Ba_2CuO_{6+\delta}$, $\odot$: $Ca_{1-x}Y_xSr_2Tl_{0.5}Pb_{0.5}Cu_2O_7$