Josephson effect as a measure of quantum fluctuations in the cuprates

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Quantitative analysis of the Josephson effect is shown to provide direct information about phase fluctuations in the superconducting banks. Applying the analysis to the cuprates, substantial quantum fluctuations between d-wave and s-wave pairing are found at low temperatures. A phenomenological model of such fluctuations is introduced and solved in a self-consistent single-site approximation. Finally we discuss the microscopic justification of the phenomenological model.

Let us first consider a toy model in which the fluctuating part \( \varphi_i \) is taken to be a random variable with the same distribution as the original phase \( \phi \). The values of \( \alpha \) determined using both types of junctions in the cuprates and solve it within the simplest nontrivial self-consistent approximation. Finally we discuss the microscopic justification of the phenomenological model.

Let us start by considering a Josephson junction described, in absence of phase fluctuations in the banks, by the harmonics \( I_n \). Now, let us switch on phase fluctuations and denote the fluctuating part of the phase in the bank \( i = 1, 2 \) as \( \varphi_i \). In the tunnel limit the phase fluctuations in different banks can be considered independent of each other. Thus at time scales longer than the typical fluctuation time and/or for junctions larger than the fluctuation correlation length, \( I(\phi) \) renormalizes to

\[
\tilde{I}(\phi) = \sum_n I_n \sin n (\phi + \varphi_1 - \varphi_2) = \sum_n \tilde{I}_n \sin n \phi,
\]

where the renormalized \( n \)-th harmonic reads \( \tilde{I}_n/I_n = \langle \cos n \varphi_1 \rangle \langle \cos n \varphi_2 \rangle \). In grain boundary junctions with a 45° misorientation between the cuprates, the first two harmonics are experimentally accessible. A detailed analysis of the data suggests that

\[
\alpha = \langle \cos \varphi \rangle \approx 0.3, \quad \beta = \langle \cos 2 \varphi \rangle \approx 1.0.
\]

We would like to point out that the value of \( \alpha \) was determined from the Josephson product \( I_R N \) of a large set of cuprate/cuprate and of cuprate/low-\( T_c \) junctions (for reviews, see) which are renormalized by \( \alpha^2 \) and \( \alpha \), respectively. The values of \( \alpha \) determined using both types of junctions in the cuprates and solve it within the simplest nontrivial self-consistent approximation. Finally we discuss the microscopic justification of the phenomenological model.

Now we proceed by introducing a minimal model of phase fluctuations consistent with Eq. (1). Our model is motivated by the strong-coupling RVB picture of the cuprates which views the cuprates as a liquid of predominantly local singlets. While the pairs are formed at a high energy scale \( \sim J \), they acquire phase coherence only at a much lower scale. Therefore we assign a fluctuating phase field \( \tilde{\varphi}_i \) to each bond \( i \) of the square Cu lattice. Note that \( \varphi_i \) is the phase of a Cooper pair, i.e. of a charge \( 2e \) object.

Let us first consider a toy model in which the fluctuating part \( \delta \varphi \) of the phase at each link is either 0 or \( \pm \pi \), with probabilities \( P_1 = (1 + \alpha)/2 \approx 0.65 \) and \( P_2 = (1 - \alpha)/2 \approx 0.35 \), respectively. One finds readily

\[
\alpha = \langle \cos \varphi \rangle \approx 0.3, \quad \beta = \langle \cos 2 \varphi \rangle \approx 1.0.
\]
that Eq. (1) is satisfied in such a model. On the other hand, Fig. 1 shows a snapshot of a typical $\phi_i$ configuration for such fluctuations. Note that the probabilities that a lattice point supports local $d$, $-d$, $s$, and $-s$ pairing symmetry are $P_1^2 \approx 0.42$, $P_2^2 \approx 0.12$, $P_1P_2 \approx 0.23$, and $P_1P_2 \approx 0.23$, respectively. In other words, the numerical values in Eq. (1) suggest the presence of strong quantum fluctuations from $d$-wave to $s$-wave pairing.

The simplest model of a superconducting CuO$_2$ plane which allows for phase fluctuations, takes into account the compact nature of the phase field, and assumes dominant $d$-wave and subdominant $s$-wave pairing (with pairing strengths $V + W$ and $V - W$, respectively), reads

$$H = -m^{-1} \sum_i \partial^2/\partial \phi_i^2 + \sum_{(i,j)} E_j(\phi_i, \phi_j).$$

(2)

The first term in Eq. (2) which allows for quantum fluctuations of phase can be thought of as a local charging energy at site $i$. Note that from now on, instead of bonds we talk about the sites of a (dual) lattice. The second term where $(i,j)$ denotes a pair of nearest neighbor sites can be viewed as a Josephson coupling between the sites $i$ and $j$, $E_j(\phi_i, \phi_j) = -V \cos(2\phi_i - 2\phi_j) + W \cos(\phi_i - \phi_j)$. Note that the sign of the $W$ term is different from the standard convention, because of the $d$-wave symmetry of pairing in the cuprates.

Let us point out that our model Eq. (2) includes the quantum XY model as a special limit $V = 0$; we will show that the most spectacular effects occur at $V \gg W$. Note also that we haven’t considered dissipative effects in Eq. (2). Since the cuprates are $d$-wave superconductors with low-lying fermionic excitations, this is a nontrivial assumption which needs to be studied in future work.

In what follows we study the model Eq. (2) by constructing a variational solution of the form

$$\psi(\phi_1, \phi_2, \ldots) = \Pi_i \psi_i(\phi_i),$$

(3)

where the product runs over all lattice sites and the local functions $\psi_i$ are $2\pi$ periodic. The Schrödinger equation for the lattice point $i$ reads

$$-m^{-1} \partial^2/\partial \phi_i^2 + U_i(\phi)\psi_i(\phi) = \varepsilon_i \psi_i(\phi),$$

(4)

with a self-consistent potential

$$U_i(\phi) = \sum_t \left[ -V \langle \cos 2\phi \rangle_{i+t} \cos 2\phi + W \langle \cos \phi \rangle_{i+t} \cos \phi \right],$$

where the sum runs over the four nearest-neighbor sites $i + t$ of the studied site and $\langle f(\phi) \rangle_i = \int d\phi f(\phi) |\psi_i(\phi)|^2$. Note that the single-site approximation Eq. (4) is similar in spirit to the self-consistent harmonic approximation, but goes beyond it by treating the local problem exactly, which is instrumental in the present context.

Now we specialize to the case of a two-sublattice solution with $\psi_i(\phi) = \psi_A(\phi)$ and $\psi_i(\phi) = \psi_B(\phi)$ for $i$ in sublattice $A$ and $B$, respectively. Note that this corresponds to a translationally invariant solution on the original lattice. Assuming furthermore a $d$-wave solution, $\psi_B(\phi) = \psi_A(\phi + \pi)$, we obtain $\langle \cos n\phi \rangle_B = (-1)^n \langle \cos n\phi \rangle_A$. The self-consistent Hamiltonian for sublattice $A$ therefore reads

$$H = -\partial^2/\partial \phi^2 - a\cos \phi - b\cos 2\phi,$$

(5)

where we have measured the energy in units of $m^{-1}$. Introducing dimensionless interaction parameters $v = mV$ and $w = mW$, the dimensionless self-consistent potentials read

$$a = 4w\alpha, \quad b = 4v\beta,$$

(6)

where $\alpha$ and $\beta$ are defined in Eq. (1) in which the mean values $\langle \phi \rangle$ are to be calculated with respect to the solution of Eq. (5). The total energy per lattice site $\bar{\varepsilon}$ differs from the lowest eigenvalue $\varepsilon$ of the Hamiltonian Eq. (5):

$$\bar{\varepsilon} = \varepsilon + (a\alpha + b\beta)/2.$$  

(7)

In Fig. 2 we plot the potential energy entering Eq. (5) in the limit $b \gg a$ relevant to the cuprates. The classical solutions at $\phi = 0$ and $\phi = \pm \pi$ are nearly degenerate, their splitting being $2a$. The ground-state wavefunction $\psi(\phi)$ is localized predominantly in the vicinity of $\phi = 0$, but tunneling across the finite barrier leads to a second peak of $\psi(\phi)$ in the vicinity of $\phi = \pm \pi$. In complete analogy with the toy model Fig. 1 this tunneling leads to quantum fluctuations between $d$-wave and $s$-wave pairing, which are thus seen to be essentially local.

Self-consistent solution to Eqs. (5,6,1) shows that three phases exist in the $w > 0$ part of the phase diagram of the model Eq. (2), see Fig. 3: (i) a conventional $d$-wave superconducting phase with $\alpha > 0$ and $\beta > 0$ realized for sufficiently large $v, w$; (ii) a quantum disordered phase with $\alpha = \beta = 0$ at small $v, w$; and (iii) an exotic superconductor phase with $\alpha = 0$ and $\beta > 0$ appearing at large $v$ and small $w$. 

FIG. 2: Solid line: Potential energy entering Eq. (5) (in arbitrary units). Result of a self-consistent calculation for $v = 1.1$ and $w = 0.09$, leading to $a \approx 0.22$ and $b \approx 2.0$. Dashed line: Square of the ground-state wavefunction $|\psi(\phi)|^2$ for the same parameters.
Extending the phase diagram for $w > 0$ to negative values of $w$, one verifies easily that the role of $d$-wave and $s$-wave pairing is interchanged and therefore the phase diagram for $w < 0$ is a mirror image of that for $w > 0$. This implies that within the quantum model Eq. (2), upon changing the sign of $W$ the superconducting state switches from $d$-wave to $s$-wave symmetry by crossing one of the two nontrivial phases in Fig. 3. Which of the two possible intermediate states is realized depends on the strength of quantum fluctuations. In the limit of strong fluctuations (small $v$), an intermediate quantum disordered state is realized [phase (ii)], which is presumably insulating. If the strength of quantum fluctuations decreases, the exotic phase (iii) separates the two conventional pairing states. In the classical limit $m \to \infty$ the width of phase (iii) vanishes. In what follows we argue that although $\cos \varphi = 0$ in phase (iii), it does represent a superconductor, albeit an exotic one, since it can be thought of as a condensate of pairs of Cooper pairs, or quadruplets of electrons [10]. Note that phase (iii) bears some similarity to the fractionalized superconductor discussed in [11].

Let us show now that phase (iii) is described by a macroscopic Ginzburg-Landau type wavefunction $\Psi_{GL}(x,y)$ with a nonvanishing phase rigidity. To this end consider the many body wavefunction Eq. (3) with the following choice of local wavefunctions,

$$\psi_{i+\hat{x}}(\varphi) = \psi_i(\varphi + \pi + \chi_1),$$

$$\psi_{i+\hat{y}}(\varphi) = \psi_i(\varphi + \pi + \chi_2),$$

where $\hat{x}$ and $\hat{y}$ are unit vectors of the lattice in the $x$ and $y$ directions, respectively. Eq. (3) corresponds to a macroscopic wavefunction with an internal $d$-wave symmetry and a spatially modulated phase $\Psi_{GL}(x,y) \propto \exp[-i(\chi_1 x + \chi_2 y)/d_0]$, where $d_0$ is the lattice constant of the dual lattice. The Schrödinger equation for site $i$ can still be written in the form of Eq. (4) with a self-consistent potential satisfying $U_{i+\hat{x}}(\varphi) = U_i(\varphi + \pi + \chi_1)$ and $U_{i+\hat{y}}(\varphi) = U_i(\varphi + \pi + \chi_2)$. The periodicity of the local wavefunctions together with Eq. (3) guarantees that all local energies $\bar{\varepsilon}_i$ are equal. For a general lattice point $i$ the potential $U_i(\varphi)$ contains terms proportional to both $\cos n\varphi$ and $\sin n\varphi$ with $n = 1, 2$. However, we assume that there exists one special lattice point for which the terms proportional to $\sin n\varphi$ vanish. For this lattice point the Hamiltonian can be written in the form of Eq. (5). The set of self-consistent equations is closed by Eq. (6), in which the effective interaction strengths $W_{\mathrm{eff}} = w(\cos \chi_1 + \cos \chi_2)/2$ and $v_{\mathrm{eff}} = v(\cos 2\chi_1 + \cos 2\chi_2)/2$ have to be used instead of $w$ and $v$, respectively. Since the total energy per lattice site is still given by Eq. (7), the energy difference between a modulated and a uniform macroscopic state can be written in a Ginzburg-Landau type form

$$\delta \bar{\varepsilon} = \bar{\varepsilon}(w_{\mathrm{eff}}, v_{\mathrm{eff}}) - \bar{\varepsilon}(w, v) \approx -\frac{\partial \bar{\varepsilon}}{\partial w} \delta w - \frac{\partial \bar{\varepsilon}}{\partial v} \delta v,$$

where $\delta w = w - w_{\mathrm{eff}} \approx w(\chi_1^2 + \chi_2^2)/4$ and $\delta v = v - v_{\mathrm{eff}} \approx v(\chi_1^2 + \chi_2^2)$ and the approximate equations are valid for slowly varying macroscopic wavefunctions, $\chi_1, \chi_2 \ll 1$. In the conventional superconductor phase [phase (i)] we expect a generic point of the phase diagram $\partial \bar{\varepsilon}/\partial w < 0$ and $\partial \bar{\varepsilon}/\partial v < 0$. From Eq. (6) it then follows that in the long-wavelength limit $\delta \bar{\varepsilon} \propto (\chi_1^4 + \chi_2^4)$, as it should be in a superconductor with a finite phase stiffness. On the other hand, in phase (iii) we have $\partial \bar{\varepsilon}/\partial w = 0$, but the inset to Fig. 4 shows explicitly that $\partial \bar{\varepsilon}/\partial v < 0$, which is enough to guarantee a finite phase stiffness in this case as well. Thus we have shown that the phase (iii) is an exotic superconductor.

Returning to the physics of cuprates, Eq. (11) implies that if we insist on their description in terms of the model Eq. (2), then its parameters should be chosen inside the phase (i), but close to phase (iii). Fig. 4 shows explicitly that in this case it is possible to have $\alpha \approx 0.3 < \beta$. Within our simplistic model it is difficult to have $\beta \approx 1$ at the same time, because this would require small quantum fluctuations (large $v$). However, for $v \gg 1$ the differ-
ence $W$ between the $d$-wave and $s$-wave pairing strengths needs to be implausibly small in order to stabilize the exotic superconductor phase.

Next we address the question whether it is reasonable to assume that, within a realistic model of the cuprates, $d$-wave and $s$-wave pairing are competitive in energy. Lead by the hypothesis that the symmetry of pairing is correctly determined already at weak coupling [12], we have studied the superconducting phase diagram of the $t$-$t'$ Hubbard model for $t'/t = 0.45$ and a moderate interaction strength $U/t = 6$ as a function of the electron density $\rho$ in the vicinity of $\rho = 0.7$. This choice of parameters is close to the canonical values for the cuprates and it is inspired by the results of [12], where a $d$-wave/$s$-wave pairing transition was found in this region.

In Fig. 5 we plot the superconducting transition temperatures determined by the variational method for a Kohn-Luttinger superconductor [13] in the two dominant pairing symmetries ($d$-wave and $s$-wave). Note that for extremely overdoped cuprates with $\rho < \rho_c \approx 0.7$, $s$-wave pairing is the leading instability. It is also shown that close to $\rho_c$, $T_c$ in the leading subdominant pairing symmetry sector ($d_{xy}$-wave) is much smaller than $T_{cd}, T_{cs}$.

According to Eq. (2), the condensation energy per site in absence of phase fluctuations is $2(V + W)$ and $2(V - W)$ in the $d$-wave and $s$-wave pairing sectors, respectively. At weak coupling, these condensation energies are proportional to $T_{cd}^2$ and $T_{cs}^2$. By comparing these expressions, we obtain a rough estimate of the coupling constants $V$ and $W$. The results are shown in Fig. 5. Note that with hole doping $x = 1 - \rho$ decreasing from $x_c \approx 0.3$ towards experimentally accessible values, both $W$ and $V$ and their ratio $W/V$ increase. On the other hand, also the fluctuations are expected to grow with underdoping, i.e. $m \to 0$ as $x \to 0$ [12, 14]. This brings us to the question about the doping dependence of $v = mV$ and $w = mW$. We hypothesize that with reduced doping, the effect of $m \to 0$ dominates and the cuprates track the line in Fig. 3 between the points OD and UD. Under further reducing the hole density, the insulating quantum disordered phase should be reached. This can happen either directly or via crossing the exotic superconductor phase, as indicated by the dashed lines in Fig. 3.

It should be remarked that the question about how $I(\phi)$ depends on the doping level is very difficult to address experimentally. An interesting possibility might be to study artificially doped grain boundary junctions [13].

In conclusion, we have found that the two seemingly independent experimental observations in the cuprates, namely the large first and the small second harmonics of the Josephson current, can be explained by a simple assumption of substantial quantum fluctuations between $d$-wave and $s$-wave pairing at low temperatures. We have introduced a phenomenological model of such fluctuations and solved it in a self-consistent single-site approximation. We have argued that the cuprate parameters lie close to an exotic superconductor phase with condensation of electron quadruplets. Finally, $d$-wave and $s$-wave pairing were shown to be competitive within the Hubbard model for parameters close to the canonical values for the cuprates.

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[1] M. Sigrist and T. M. Rice, J. Phys. Soc. Jpn. 61, 4283 (1992).
[2] C. C. Tsuei and J. R. Kirtley, Rev. Mod. Phys. 72, 969 (2000).
[3] K. K. Likharev, Rev. Mod. Phys. 51, 101 (1979).
[4] R. Hlubina, M. Grajcar, and E. Iliechev, preprint cond-mat/0211255.
[5] R. Hlubina, preprint cond-mat/0210516.
[6] P. W. Anderson, Science 235, 1196 (1987).
[7] H. Hilgenkamp and J. Mannhart, Rev. Mod. Phys. 74, 485 (2002).
[8] S. Chakravarty et al., Phys. Rev. B 37, 3283 (1988).
[9] P. A. Lee and X. G. Wen, Phys. Rev. Lett. 78, 4111 (1997).
[10] For nonlocal pairs $b_{ij} = (c_i^\dagger c_j^\dagger - c_i^\dagger c_j^\dagger)/\sqrt{2}$, quadruplet condensation is possible since $(b_{ij})^2 = -c_i^\dagger c_i^\dagger c_j^\dagger c_j^\dagger$.
[11] T. Senthil and M. P. A. Fisher, Phys. Rev. B 62, 7850 (2000).
[12] R. Hlubina, Phys. Rev. B 59, 9600 (1999).
[13] J. Mráz and R. Hlubina, preprint cond-mat/0212176.
[14] Y. J. Uemura et al., Phys. Rev. Lett. 62, 2317 (1989).
[15] G. Hammerl et al., Nature (London) 407, 162 (2000).