Josephson scanning tunneling microscopy.

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We propose a set of scanning tunneling microscopy experiments in which the surface of superconductor is scanned by a superconducting tip. Potential capabilities of such experimental setup are discussed. Most important anticipated results of such an experiment include the position-resolved measurement of the superconducting order parameter and the possibility to determine the nature of the secondary component of the order parameter at the surface. The theoretical description based on the tunneling Hamiltonian formalism is presented.

I. INTRODUCTION

Recent technological advances allowed Pan et al. to conduct very low temperature scanning tunneling microscopy (STM\textsuperscript{[1]} experiments reaching temperatures as low as 220 mK and making possible the direct imaging of the surface of high-$T_c$ superconductors (SC) in a superconducting state with high spatial and energy resolution.\textsuperscript{[2]} The Pt/Ir tips used in these experiments were not superconducting, but the same group has reported earlier\textsuperscript{[3]} that they were able to obtain the atomic resolution images of superconducting NbSe\textsubscript{2} with the superconducting atomically sharp Nb tip in the quasiparticle tunneling regime. The idea of STM experiment in which the Josephson effect would be observed between the tip and the surface was also suggested.\textsuperscript{[4]}

If both the tip and the surface are superconducting and the temperature is low enough to have a well-defined phase difference between the superconductors, the tunneling contact may be considered a Josephson junction with tunable parameters (hence the term “Josephson STM” or JSTM). The phase-dependent supercurrent will not be washed out by thermal fluctuations if the temperature is sufficiently low,

\[ I_c \Phi_0 \geq 2 \pi k_B T, \]  

where $I_c$ is the critical Josephson current and $\Phi_0 = \hbar/2e$ is the unit magnetic flux. Assuming that the Josephson current can be roughly estimated as $I = s \Delta/e$,\textsuperscript{[5]} where $\Delta$ is the magnitude of the superconducting order parameter (OP) and $s$ is the normal state conductance of the junction, Eq. (1) translates into the condition imposed on the normal state resistance:

\[ R \leq \frac{\Delta}{2k_B T} R_0. \]  

Here $R_0 = \hbar/e^2 \approx 4$ kΩ is the resistance quantum. For conventional superconductors ($\Delta \sim 2$ meV) and temperature $T \sim 0.1$ K the junction resistance should not exceed $\sim 500$ KΩ for the Josephson current to be observable. For higher gap values, such as in high-$T_c$ materials, we estimate $R \leq 7.5$ MΩ. Since the temperature enters into criteria (3) only via ratio $\Delta/kT$, it might be easier to observe Josephson current using high-$T_c$ material with a larger value of $\Delta$ as a tip rather than to lower temperature by an order of magnitude.

Typical resistances of STM experiments are at least by an order of magnitude larger, than the estimated upper bounds for Josephson effect. Thus, Josephson supercurrent is difficult to observe in a setup with an atomically sharp superconducting tip. Therefore we propose the use of a tip with a finite tunneling area. While it will be impossible to achieve the atomic-scale spatial resolution, to capture the microscopic variations of superconducting OP only the resolution comparable to the coherence length of SC is needed. This characteristic length is about 20 Å for the high-$T_c$ materials and a few thousand Å for conventional superconductors. Also, the finite tunneling area will lead to relatively big capacitance of the junction, minimizing the charging energy and making the effects of Coulomb blockade negligible.

Since the supercurrent depends on the magnitudes of the superconducting OP on both sides of the junction,\textsuperscript{[6]} it should be possible to measure the microscopic variations in OP depending on the position of the tip. Such measurement can provide a direct insight into the microscopic nature of the superconducting state.

Another potential application of the JSTM is the probing of the symmetry of superconducting OP. It is known that a perturbation, such as an applied magnetic field or a surface, can induce a secondary component of the superconducting OP. The type of the secondary component can be determined from the modification of the Josephson current. In case when both the tip and the surface are unconventional superconductors, like high-$T_c$ cuprates, the OP is angle-dependent and the variations in the tunneling supercurrent may be caused by changing the mutual orientation, providing the direct information about the symmetry of OP.

Finally, the JSTM could provide information about the nature of the gap in high-$T_c$ superconductors. It is believed, that the normal state of the underdoped high-$T_c$ cuprates is a pseudogap (PG) state with partially gapped Fermi surface, from which superconductivity emerges as the temperature is lowered through $T_c$.\textsuperscript{[7]}

Currently there is no general agreement on the origin of PG state. Some models attribute PG to superconducting phase fluctuations above $T_c$.\textsuperscript{[8]} Others\textsuperscript{[9]} to a competing non-superconducting order parameter.\textsuperscript{[10]} Since JSTM...
is sensitive only to the superconducting OP, the measurements of the critical Josephson current on differently doped samples can shed some light on the origin of PG.

The rest of the paper is organized as follows: in Section II we describe the tunneling Hamiltonian formalism used in the calculations and two practically important cases of JSTM, followed by proposed experimental setup (Section III) and summary (Section IV).

II. THEORETICAL DESCRIPTION

We base our theoretical description of JSTM on the tunneling Hamiltonian formalism. In this formalism, time-dependent Josephson current through the tunneling contact is expressed as

$$I_J(t) = 2e \text{Im} \{ \exp(-2ieVt/\hbar) \Phi_{\text{ret}}(eV) \},$$

where $V$ is the applied voltage and $\Phi_{\text{ret}}(eV)$ is the voltage-dependent retarded correlation function, which in the limit of the zero temperature has the form

$$\Phi_{\text{ret}}(eV) = \frac{1}{2} \sum_{kp} T_{kp} T_{-k,-p} \frac{\Delta_k \Delta_p}{E_k E_p} \times \left( \frac{1}{eV + E_k + E_p + i\delta} - \frac{1}{eV - E_k - E_p + i\delta} \right).$$

Here indices $k$ and $p$ refer to the quasiparticle momenta of the tip and surface, respectively, $T_{kp}$ is the tunneling matrix element, $\Delta_k$ and $\Delta_p$ are the superconducting order parameters, $E_k$ and $E_p$ are the excitation energies, and the infinitesimal quantity $i\delta$ ensures the convergence of the integral.

Using Eqs. (3) and (4) we can calculate the Josephson current for a tunneling contact of two superconductors. Unique feature of the Josephson effect is that below a certain threshold value, the dc supercurrent can flow without any voltage drop on the contact. This threshold value – critical Josephson current – is easily measured, because when the value of the current reaches the critical value, the finite voltage drop abruptly appears at the contact. If the analytical expression for the critical current is known, its measurements can provide the information about the magnitudes of OPs, its symmetry and possibly other quantities of interest.

A. s-d junction

First we consider the case when the STM tip is a conventional s-wave SC (superconducting metal, like Nb) with momentum-independent real order parameter $\Delta_k \equiv \Delta_1$ and the surface under study is the $a$-$b$ plane of a $d$-wave unconventional SC (e.g., YBCO or BSCCO). It is generally agreed, that perturbation of the unconventional $d$-wave superconductors, like magnetic field or the distortion of crystal lattice caused by presence of the surface, induces a secondary component of the superconducting OP. Tuning between pure $s$- and $d$-wave superconductors is expected to be zero by symmetry arguments, at least if one does not take into account the higher order processes. Experimental evidence exists that the secondary component in high-$T_c$ cuprates possesses $s$-wave symmetry. In order to determine the dependence of the critical Josephson current both on the magnitude and the phase of the secondary OP component, we have chosen the following form for the superconducting OP on the surface:

$$\Delta_p = \Delta_2 = \Delta_2^{(d)} \cos 2\varphi + e^{i\alpha} \Delta_2^{(s)}.$$  

Here $\Delta_2^{(d)}$ and $\Delta_2^{(s)}$ are the magnitudes of the primary and secondary components (respectively) and $\varphi$ is the azimuthal angle corresponding to momentum $p$ in the coordinate system associated with the surface plane. By varying angle $\alpha$ the secondary component can be assigned an arbitrary phase: In particular $\alpha = 0$ corresponds to pure $d + s$ symmetry and $\alpha = \pi/2$, to $d + is$. The excitation energies $E_k$ and $E_p$ are given by familiar relations

$$E_k = \sqrt{\xi_k^2 + \Delta_1^2},$$

and

$$E_p = \sqrt{\xi_p^2 + |\Delta_2|^2},$$

where $\xi_k$ and $\xi_p$ are the single-particle energies, measured with respect to corresponding chemical potentials. We assume here that the tunneling matrix element is independent of momenta, i.e.

$$T_{kp} T_{-k,-p} = |T|^2 e^{i\phi}.$$  

Here $|T|^2$ is a constant, depending only on the geometry of the tunneling contact (it drops exponentially with increasing distance between tip and the surface) and $\phi$ is the phase difference, giving rise to Josephson supercurrent.

In order to calculate the sums in Eq. (6), we convert them into integrals over the energies $\xi_k$, $\xi_p$ and the azimuthal angle $\varphi$. In the case of zero applied voltage, the integral with respect to energies can be calculated using the result due to Ambegaokar and Baratoff to yield

$$\Phi_{\text{ret}}(0) = \frac{\sigma_0}{2\pi e^2} \int_0^{2\pi} \frac{\Delta_1 \Delta_2}{\Delta_1 + |\Delta_2|} K \left( \frac{|\Delta_1 - |\Delta_2||}{\Delta_1 + |\Delta_2|} \right) d\varphi$$  

(9)

Here $K(x)$ is the complete elliptic integral of the first kind and $\sigma_0$ is the conductance of the tunneling contact in the normal state.

$$\sigma_0 = 4\pi e^2 N_1 N_2 |T|^2$$  

with $N_1$ and $N_2$ being the densities of states at the Fermi levels of tip and surface respectively. The critical Josephson current in this case is

$$I_c = I_c^0 |\chi(\gamma, \kappa, \alpha)|,$$  

(11)
where $\gamma = \Delta_2^{(d)}/\Delta_1$ and $\kappa = \Delta_2^{(s)}/\Delta_1$ are dimensionless parameters, $F_0^c = \Delta_1\sigma_0/e\pi$ and $\chi(\gamma, \kappa, \alpha)$ is the value of integral in Eq. (1). Assuming, that $\Delta_1$ is fixed, we have studied numerically the dependence of the critical current on $\gamma$, $\kappa$ and $\alpha$ for realistic parameter ranges.

The dependence of the critical Josephson current for $\alpha = 0$ (corresponds to pure $d+s$ symmetry) on $\gamma$ and $\kappa$ is shown on Fig. 1.

Another important case is $\alpha = \pi/2$, which corresponds to $d+is$ symmetry of superconducting OP. The results for this case are presented in Fig. 2.

![Fig. 1](image1.png)

**FIG. 1.** The dependence of the critical Josephson current on $\gamma$ and $\kappa$ for an $s$-$d$ junction in the limit of zero applied voltage and $\alpha = 0$. Different curves correspond to different values of $\kappa$, starting from $\kappa = 0.01$ (lowest curve) with the increment of 0.01. The uppermost curve thus corresponds to $\kappa = 0.1$.

![Fig. 2](image2.png)

**FIG. 2.** The dependence of the critical Josephson current on $\gamma$ and $\kappa$ for an $s$-$d$ junction in the limit of zero applied voltage and $\alpha = \pi/2$. Different curves correspond to different values of $\kappa$, starting from $\kappa = 0.01$ (lowest curve) with the increment of 0.01. The uppermost curve thus corresponds to $\kappa = 0.1$.

Useful information can also be extracted from the observation of quasiparticle current between superconductors at a finite temperature. The current can be written as:

$$I = \frac{\sigma_0}{2\pi e} \int_0^{2\pi} d\varphi \int_{-\infty}^{+\infty} \frac{|E|}{\sqrt{E^2 - \Delta_1^2}} \frac{|E + eV|}{\sqrt{(E + eV)^2 - |\Delta_2|^2}} [f(E) - f(E + eV)] dE,$$

where $f(E)$ is a Fermi-Dirac distribution function and the regions $|E| < \Delta_1$ and $|E + eV| < |\Delta_2|$ are excluded from the integration. We have numerically calculated current-voltage characteristic for a realistic set of parameters: $\Delta_1/kT = 2$, $\Delta_2^{(d)}/\Delta_1 = 10$ and $\Delta_2^{(s)}/\Delta_2^{(d)} = 0.025$. It is known from Eq. (5) that when the tunneling contact of two $s$-wave superconductors with different constant real order parameters $\Delta_1$ and $\Delta_2$ is considered, the quasiparticle current-voltage characteristic possesses two significant features: a peak at the voltage $|\Delta_1 - \Delta_2|$ and an abrupt increase in current at voltage $\Delta_1 + \Delta_2$, corresponding to transition to Ohmic regime. We find that the position of the peak and the Ohmic transition depends on the symmetry of the superconducting OP. In particular (as seen in Fig. 3) the current is sharply peaked at the voltage $\Delta_2^{(d)} - \Delta_1$ for $\alpha = \pi/2$ ($d+is$ symmetry), while for $\alpha = 0$ the peak is at the voltage $\Delta_2^{(d)} + \Delta_2^{(s)} - \Delta_1$. The transition to Ohmic regime is also shifted to higher voltages by the value of $\Delta_2^{(s)}$. Thus, such a measurement can complement the measurements of Josephson critical current to provide additional information about the nature and magnitude of superconducting OP on the surface.

![Fig. 3](image3.png)

**FIG. 3.** Typical quasiparticle current-voltage characteristic (values of parameters are given in the text) of a tunneling contact between $d$-wave superconductor with the secondary OP component and $s$-wave superconductor. Different values of $\alpha$ correspond to $d+s$ ($\alpha = 0$) and $d+is$ ($\alpha = \pi/2$) symmetries.
B. d-d junction

The d-wave nature of a pair requires finite size tunneling area. If the tunneling occurs from only one site on the tip it would imply effective momentum averaging of pair wavefunction and would yield zero Josephson current for d-wave pairs. Thus it is desirable to have a finite region of the tip where tunneling can occur. In this case, one loses spatial resolution, compared to conventional tips. However the gain is the phase coherent current between the tip and the surface. While the idea of using the high-\(T_c\) cuprates as a material of STM tip has not yet been reported in the literature, the fabrication of relatively small (of the order 100 Å) flat high-\(T_c\) probes, suitable for use (as tips), is feasible.

Theory based on tunneling Hamiltonian predicts, that if the tunneling matrix element is momentum-independent, c-axis Josephson current at zero temperature is identically zero for superconductors with pure d-wave symmetry of OP. It is possible to argue that, as discussed in previous section, the presence of the surface will induce the secondary OP component, which can lead to a nonzero current. However, since the magnitude of secondary component is usually much smaller than the magnitude of primary one, this induction will produce a second order effect and we assume that it can be neglected.

\[
\Delta_1 = \Delta_1^{(0)} \cos 2\varphi
\]

and

\[
\Delta_2 = \Delta_2^{(0)} \cos (2(\varphi + \theta)).
\]

Tunneling matrix element has the form

\[
T_{k\mathbf{p}} T_{-k\mathbf{p}} = |T|^2 e^{i\varphi} \delta(k - \mathbf{p}),
\]

where \(k\) and \(\mathbf{p}\) are two-dimensional vectors. Again, we change the sums in Eq. (3) into integrals, which can be calculated numerically. In the case of zero applied voltage and zero rotation angle \(\theta\) it is possible to calculate the integral analytically and find that the critical Josephson current in this limit is

\[
I_c = I_c^0 \frac{\gamma \ln \gamma^2}{\gamma^2 - 1},
\]

where \(\gamma = \Delta_1^{(0)}/\Delta_2^{(0)}\), assuming \(\Delta_1^{(0)} < \Delta_2^{(0)}\), and \(I_c^0\) is constant current independent of \(\gamma\). This dependence is presented in Fig. 4. \(\gamma = 0\) corresponds to absence of the superconductivity in the tip, which leads to disappearance of the Josephson current.

We have also studied the dependence of the critical current on the rotation angle \(\theta\) at zero applied voltage (Fig. 5). As expected, it has a maximum at \(\theta = 0\), monotonically decreases with increasing \(\theta\) and becomes zero at \(\theta = \pi/4\). For the angles bigger than \(\pi/4\), the critical current can be obtained as

\[
I_c \left(\frac{\pi}{4} + \theta\right) = -I_c \left(\frac{\pi}{4} - \theta\right),
\]

i.e. for \(\theta > \pi/4\) the current changes direction, but the curve remains symmetric with respect to the point \(\theta = \pi/4\). It is notable, that since the curve is symmetric with respect to \(\theta = 0\), there is a kink in the angle dependence at \(\theta = 0\).

The problem is essentially two-dimensional and the order parameters of the tip \(\Delta_1\) and surface \(\Delta_2\) may be used.

\[
I_c = I_c^0 \frac{\gamma \ln \gamma^2}{\gamma^2 - 1} \left(1 - \frac{4}{\pi} \theta\right)
\]



FIG. 4. The dependence of the critical Josephson current on the ratio of OP magnitudes for a d-d junction in the limit of zero applied voltage and zero rotation.

Here we discuss a different scenario, supported by recent theoretical and experimental work of Latyshev et al. In their work, the intrinsic c-axis quasiparticle transport between layers of BSCCO was studied. It was found that interlayer transport is predominantly momentum-conserving, i.e. the in-plane components of quasiparticle momentum are conserved in the tunneling process. It seems natural to make an assumption, that in-plane momentum is also conserved in case of Josephson supercurrent. As we show below, adoption of this hypothesis leads to non-zero current even in the case of pure d-wave symmetry.

We consider an a-b plane tunneling contact of two d-wave superconductors. We allow the magnitudes of the superconducting OP to be different. Because of the angular dependence of the superconducting OP, the Josephson current will depend on the mutual orientation of two superconductors and we introduce angle \(\theta\) (angle between a-axes of superconductors) to describe this orientation. The problem is essentially two-dimensional and the order parameters of the tip \(\Delta_1\) and surface \(\Delta_2\) may be written as

\[
\Delta_1 = \Delta_1^{(0)} \cos 2\varphi
\]

and

\[
\Delta_2 = \Delta_2^{(0)} \cos (2(\varphi + \theta)).
\]

The problem is essentially two-dimensional and the order parameters of the tip \(\Delta_1\) and surface \(\Delta_2\) may be written as

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\Delta_1 = \Delta_1^{(0)} \cos 2\varphi
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and

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\Delta_2 = \Delta_2^{(0)} \cos (2(\varphi + \theta)).
\]

Tunneling matrix element has the form

\[
T_{k\mathbf{p}} T_{-k\mathbf{p}} = |T|^2 e^{i\varphi} \delta(k - \mathbf{p}),
\]

where \(k\) and \(\mathbf{p}\) are two-dimensional vectors. Again, we change the sums in Eq. (3) into integrals, which can be calculated numerically. In the case of zero applied voltage and zero rotation angle \(\theta\) it is possible to calculate the integral analytically and find that the critical Josephson current in this limit is

\[
I_c = I_c^0 \frac{\gamma \ln \gamma^2}{\gamma^2 - 1},
\]

where \(\gamma = \Delta_1^{(0)}/\Delta_2^{(0)}\), assuming \(\Delta_1^{(0)} < \Delta_2^{(0)}\), and \(I_c^0\) is constant current independent of \(\gamma\). This dependence is presented in Fig. 4. \(\gamma = 0\) corresponds to absence of the superconductivity in the tip, which leads to disappearance of the Josephson current.

We have also studied the dependence of the critical current on the rotation angle \(\theta\) at zero applied voltage (Fig. 5). As expected, it has a maximum at \(\theta = 0\), monotonically decreases with increasing \(\theta\) and becomes zero at \(\theta = \pi/4\). For the angles bigger than \(\pi/4\), the critical current can be obtained as

\[
I_c \left(\frac{\pi}{4} + \theta\right) = -I_c \left(\frac{\pi}{4} - \theta\right),
\]

i.e. for \(\theta > \pi/4\) the current changes direction, but the curve remains symmetric with respect to the point \(\theta = \pi/4\). It is notable, that since the curve is symmetric with respect to \(\theta = 0\), there is a kink in the angle dependence at \(\theta = 0\).

It can be seen from Fig. 5 that the decrease is almost linear with \(\theta\) and linear approximation becomes better as \(\gamma\) is reduced. For practical purposes an approximate formula

\[
I_c = I_c^0 \frac{\gamma \ln \gamma^2}{\gamma^2 - 1} \left(1 - \frac{4}{\pi} \theta\right)
\]

may be used.
FIG. 5. The dependence of the critical Josephson current on the rotation angle $\theta$ for a $d$-$d$ junction in the limit of zero applied voltage at different values of $\gamma$ (solid lines). Dashed lines show the linear approximation of Eq. (18).

It is worth mentioning that when the angle $\theta$ is non-zero, the denominator in Eq. (4) has a positive lower bound. This means that for voltages much smaller than this lower bound, the integrand may be expanded in powers of voltage. It turns out that all first order terms in voltage exactly cancel out and dependence on voltage enters only as higher order corrections (proportional to the square of the voltage), so the zero-voltage behavior is not altered significantly. The range of applicability of this approximation depends on actual values of $\gamma$ and $\theta$.

### III. EXPERIMENTAL SETUP

The sketches of experimental setup for $s$-$d$ and $d$-$d$ tunneling are shown in Fig. 6 and Fig. 7 respectively. In both cases, superconducting tip and surface form an electric circuit together with current (voltage) source and measuring equipment.

FIG. 6. Proposed experimental setup for $s$-$d$ tunneling.

In $s$-$d$ case, measurements can be performed in two stages. First, by driving a large current through the tunneling contact, the superconductivity is suppressed and the normal state conductance of the tunneling junction at the specific position on the surface is measured. Next, the measurement of the critical Josephson current (by starting with zero current and increasing it until a voltage drop appears on the contact) is performed. Using this information, a conclusion can be made about the magnitudes of the primary and/or secondary OP components on the surface. By repeating the measurement, a surface map of variations in order parameter may be obtained. Both the surface, formed by $a$-$b$ plane and the one, parallel to $c$-axis can be studied.

FIG. 7. Proposed experimental setup for $d$-$d$ tunneling.

In $d$-$d$ case, the apparatus must be designed in such a way that the tip can be rotated around vertical axis. Measuring the Josephson current as a function of rotation angle, the information about the symmetry of OP can be extracted. If Josephson current has nodes, separated by $\Delta \theta = \pi/2$, a conclusion can be made that the non-zero Josephson current is due to coherent tunneling and superconductors possess pure $d$-wave symmetry. If, on the other hand, current never becomes zero or becomes zero with different periodicity, then the secondary component of the OP must be a primary reason for the existence of the current.

Finally, the experiments aimed at establishing the nature of the pseudogap should be conducted with differently doped tip and surface. For example, measuring critical Josephson current in a setup with underdoped tip and overdoped surface and comparing it with measurements on identically underdoped (or overdoped) contacts will provide information about the magnitude of the pseudogap and whether or not it is of superconducting origin. Detailed discussion of such an experiment will be given elsewhere.

### IV. SUMMARY

In summary, we have a proposed a series of STM experiments of a superconducting surface with a superconducting tip. Treating the tunneling contact as a Josephson junction with tunable parameters, we have developed a theoretical description of these experiments, calculating...
the dependence of critical Josephson current on various relevant parameters. Since Josephson current is sensitive to the magnitudes of superconducting order parameters in the tip and in the surface, this new technique allows to measure the microscopic spatial variations of the OP on the surface and determine the magnitude and phase of the secondary OP component, induced by the surface. It is also possible to probe the symmetry of superconducting OP directly, exploiting the dependence of the Josephson critical current on the mutual orientation of \( d \)-wave superconductors. Finally, since the Josephson current is sensitive only to the superconducting gap, the new technique can provide information about the nature of the pseudogap, in particular, confirm or falsify its superconducting origin.

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