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Mechanisms of superconductivity studied by two-particle emission

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Abstract

It is shown theoretically that the one-photon two-electron emission spectroscopy of superconducting surfaces provides novel information on the mechanisms of superconductivity. In particular, measured angular correlations of the photo-excited (Cooper) pairs can be related to the Cooper pair wave function in momentum space. We outline how the use of circularly polarized photons gives access to phase properties of the superconducting gap function. Furthermore, we discuss the influence of the topology of the sample and the influence of an external magnetic field for the case of superconducting rings pierced by a magnetic flux.

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1. Introduction

According to Landau's theory of Fermi liquids, the electronic properties of normal metals can be understood in terms of independent quasiparticles with a well-defined energy–momentum dispersion relation [1]. In many cases however, this picture is not viable: inter-quasiparticle interactions result in an instability of these liquids and new phases of matter emerge. Prominent examples are ferromagnetism and superconductivity [2,3]. This contribution focuses on superconductivity and how the underlying mechanism can be studied by means of photo-induced coincident two-particle emission [4–6]. While the underlying physics of conventional weak-coupling superconductors (SCs) is well described by the Bardeen–Cooper–Schrieffer (BCS) [7–9] theory, the appropriate mechanisms of high-temperature superconductivity (HTSC) [10] are still under discussion (cf. [11,12] and references therein). For example, triplet p-wave SCs such as layered Sr_2RuO_4 compounds [3] are believed to exhibit a time-reversal symmetry break [13], meaning that the superconducting state, also called the chiral or the Anderson–Brinkmann–Morel (ABM) state [2,3], is not invariant under time-reversal.

On the experimental side, the magnitude, the symmetry and the temperature dependence of the superconducting gap function have been investigated by means of a variety of experimental techniques, such as the neutron and the polarization-resolved Raman spectroscopy [14,15], the infrared photoabsorption spectroscopy [16], the de Haas–van Alphen effect [17], the scanning tunneling spectroscopy [18–20], and the single photoemission spectroscopy (PES) [21,22] where in the superconducting state an energy gap $2\Delta(T)$ (centered around the Fermi level E_F) occurs in the photoelectron energy spectrum.

In double photoemission (DPE), the topic of this work, PES is extended as to detect two electrons emitted upon one-photon absorption allowing thus for a direct insight into the angular and/or energy pair correlation within the momentum–space pair function. In addition, we discuss how the measurement of the circular dichroism can be utilized to access phase information of the order parameter and to explore the role of topology by studying superconducting rings.

2. Theoretical overview

In DPE, a photon with energy ω is absorbed by a SC sample and two electrons with energies $E_{1/2}$ (relative to the chemical potential) escape the surface under the angles $\theta_{1/2}$. The DPE

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current J_{12} is written as [4]

$$J_{12} \propto \langle \Psi^{(-)}_{p_1 p_2} | D_{12} A^{(-)}_{12}(E_{12}) D^{\dagger}_{12} | \Psi^{(-)}_{p_1 p_2} \rangle = \sum_{k_1 k_2 k_1' k_2'} M_{k_1,k_2} M^{\dagger}_{k_1',k_2'} A^{(-)}_{12}(k_1 k_2 k_1' k_2'; E_{12}). \quad (1)$$

Here $p_j \equiv \mathbf{p}_j \sigma_j$ labels the state of the electron j with the electron wave vector $\mathbf{p}_j$ and spin σ_j. The matrix elements M_{k_1,k_2}, given by

$$M_{k_1,k_2} = \langle \Psi^{(-)}_{p_1 p_2} | D_{12} | k_1 k_2 \rangle, \quad (2)$$

are expressed in a spinor plane wave basis $|k_1 k_2\rangle \equiv |k_1\rangle \otimes |k_2\rangle$. In Eq. (1), $E_{12} = E_1 + E_2 - \omega$ is the binding energy of the occupied two-electron state, and $D_{12} = (A/c)[\mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{r}_1} \hat{\boldsymbol{\epsilon}} \cdot \underline{\mathbf{p}}_1 + \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{r}_2} \hat{\boldsymbol{\epsilon}} \cdot \underline{\mathbf{p}}_2]$ is the coupling operator of the photon to the electron-pair. $\mathbf{A}$ is the vector potential, $\hat{\boldsymbol{\epsilon}}$ is a polarization vector, and $\mathbf{q}$ is a wave number. c is the light velocity and $\underline{\mathbf{p}}_{1/2}$ are the one-electron momentum operators. The correlated photoelectron pair state $|\Psi^{(-)}_{p_1 p_2}\rangle$ is obtained by back-propagating (in the presence of the crystal potential) the asymptotic (detected) pair state $|p_1 p_2\rangle$ by means of the particle–particle propagator. $A^{(-)}_{12}$ is the hole–hole spectral function. For conventional SC at temperatures $T < T_\mathrm{c}$, the BCS theory yields

$$A^{(-)}_{12}(k_1 k_2 k_1' k_2'; E_{12}) = \int \frac{\mathrm{d}t}{2\pi} \mathrm{e}^{-\mathrm{i}E_{12}t} \langle\langle c^{+}_{k_1'}(t) c^{+}_{k_2'}(t) c_{k_2} c_{k_1} \rangle\rangle, \quad (3)$$

where $c^{+}_{k}(t)[c_k(t)]$ is the Heisenberg creation [annihilation] operators. To evaluate the thermodynamical average $\langle\langle \cdots \rangle\rangle$, one utilizes the Bogoliubov operators $\alpha^{+}_{k}(t) = \mathrm{e}^{\mathrm{i}E_k t} \alpha^{+}_{k}$ [$\alpha_k(t) = \mathrm{e}^{-\mathrm{i}E_k t} \alpha_k$] that create [annihilate] an elementary excitation (Bogolon) with energy $E_k = \sqrt{\varepsilon_k^2 + \Delta_k^2(T)}$, where ε_k is the excitation energy in the normal state and $\Delta_k(T)$ is the energy gap in the SC state. Using the unitary transformation

$$c^{+}_{k} = u_k \alpha^{+}_{k} + v_k \alpha_{-k} \quad (4)$$

where the expansion (also called coherence) factors satisfy the relations

$$v_k^2 + u_k^2 = 1, \quad v_k^2 = \frac{1}{2}\left[1 - \frac{\varepsilon_k}{E_k}\right], \quad u_k v_k = \frac{\Delta_k(T)}{2E_k}$$

and integrating over the time variables, one finds [4]

$$A^{(-)}_{12}(k_1 k_2 k_1' k_2'; E_{12}) = A^{(-)}_{\mathrm{UP}}(E_{12}) + A_{\mathrm{CP}}(E_{12}). \quad (5)$$

$A^{(-)}_{\mathrm{UP}}$ describes two independent Bogolons and its explicit form is given in Ref. [4]. The DPE photocurrent associated with the condensed Cooper pairs (CPs) is

$$A_{\mathrm{CP}}(E_{12}) = \delta_{k_1,-k_2} \delta_{k_1',-k_2'} \frac{\Delta_{k_1}(T) \Delta_{k_1'}(T)}{4 E_{k_1} E_{k_1'}} \delta(E_{12}). \quad (6)$$

We note that $\Delta_k(T)/2E_k$ is the wave function of CP in momentum space, when transformed into real space it is then called the order parameter in the Landau–Ginzburg theory. Hence, $A_{\mathrm{CP}}(E_{12})$ vanishes above T_c. The relation of A_{CP} to the pairing mechanism is revealed by recalling that

$$\Delta_k = \frac{1}{2} \sum_{k'} V(k, k') \frac{\Delta_{k'}}{E_{k'}},$$

where $V(k, k')$ is the pairing potential. Hence, the two-electron photocurrent can be written as $J_{\mathrm{UP}} + J_{\mathrm{CP}}$ and is relatable to the pairing mechanism. The only prerequisite on the SC for the above derivation to be valid is the existence of an underlying pairing mechanism. No assumptions are made as to the specific structure of the order parameter.

Additional information can be obtained by measuring the circular dichroism (CD), which is the normalized difference between the DPE currents resulting from left and right circular polarized photons, i.e.,

$$\mathrm{CD} = \frac{\sum_i (|M_{\hat{\epsilon}}|^2 - |M_{\hat{\epsilon}*}|^2) \delta(E_1 + E_2 - E_i - \omega)}{\sum_i (|M_{\hat{\epsilon}}|^2 + |M_{\hat{\epsilon}*}|^2) \delta(E_1 + E_2 - E_i - \omega)}.$$

As shown in detail in Refs. [5,6], if we write the complex gap function as $\Delta = |\Delta| \mathrm{e}^{\mathrm{i}\chi}$ then CD becomes proportional to the gradient of χ, more precisely

$$\mathrm{CD} \propto \mathbf{q}_{||} \cdot \nabla_{\mathbf{p}_{||}} \chi_{\mathbf{p}_{||}},$$

where $\mathbf{q}_{||}$ and $\mathbf{p}_{||}$ are, respectively, the surface parallel components of the photon wave vector and the relative momentum of the electron pair.

3. Numerical illustrations

3.1. S-wave pairing

For numerical realization, we assume the matrix elements to be almost constant on the scale of few Δ's and adopt, as done in the single photoelectron spectroscopy [22], a free-electron model for the normal state. At first we consider the s-wave pairing, i.e., $\Delta_k(0) = \Delta_0 \theta(\omega_\mathrm{D} - |\varepsilon_k|)$, where ω_D is the Debye frequency. In Fig. 1 we present the results for the DPE spectrum. The position ($E_{12} = 0$) and magnitude of the peak in the DPE current from pairing states reflect, respectively, the condensation and the (macroscopic) number of Cooper pairs in the system. Above T_c the contribution J_{CP} to the DPE current diminishes and only the uncorrelated DPE current J_{UP} is present. We note however that below T_c the contribution J_{UP} is, nevertheless, modified due to the opening of a gap in the one-electron density of states. Comparing PES and DPE results shown in Fig. 1(a and b), we conclude that the DPE current carries qualitatively different information, manifested in the behaviour that a peak at $E_{12} = 0$ occurs instead of a shift $E_{12} < 0$ as in PES. This is because in PES the photon absorption results in an unpaired hole in the supercondensate. In contrast, in DPE the photon creates two paired holes.

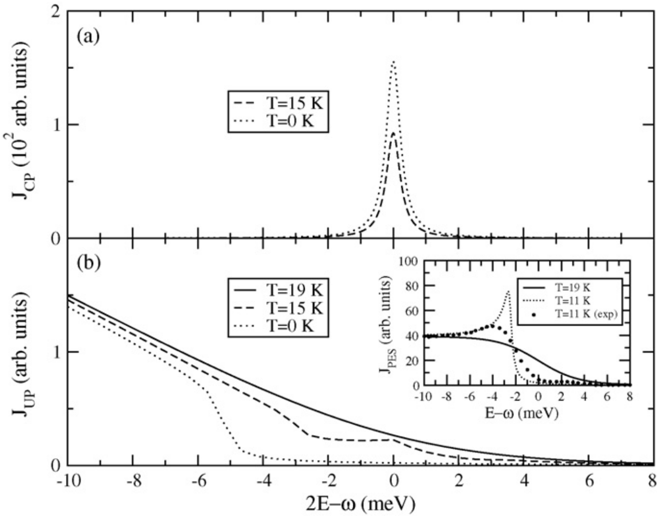

Fig. 1. DPE current as a function of the energy $2E-\omega=E_{12}$ and the temperature T. The sample is V_3Si which has the parameters: $\Delta_0=2.6$ meV, and $T_c=17$ K. (a) and (b) show J_{CP} and J_{UP}. The inset in (b) shows theoretical and experimental results [22] for the angle-integrated single photoemission. The theory does not account for the experimental resolution.

3.2. CuO_2 materials

Now we turn to the case of HTSC materials. While the precise mechanism of superconductivity in this case is still debated, evidence indicates that pairing plays as well a role. For example, for copper oxide HTSC materials a $d_{x^2-y^2}$ wave pairing symmetry in CuO_2 planes has been suggested [23], i.e.,

$$\Delta_k=\Delta_{x^2-y^2}[\cos(k_xa)-\cos(k_ya)]. \tag{7}$$

Here a is the lattice constant. As usually realized in angle-resolved single-electron photoemission studies on HTSC materials [24], we take the CuO_2planes to be parallel to the surface. The SC gap (7) is a real function. Hence, the circular dichroism vanishes. On the other hand, the admixture of s-wave pairing symmetry results in [25,26] the gap function

$$\Delta_k=\Delta_{x^2-y^2}[\cos(k_xa)-\cos(k_ya)]+\mathrm{i}\Delta_s$$

which shows a circular dichroic effect, namely

$$\mathrm{CD(CP)}\propto\frac{\Delta_{x^2-y^2}\Delta_s[aq_x\sin(p_xa)-aq_y\sin(p_ya)]}{\Delta^2_{x^2-y^2}[\cos(p_xa)-\cos(p_ya)]^2+\Delta_s^2}.$$

Note that an experimental evidence for a circular dichroic effect will indicate a pairing mechanism that breaks time symmetry. For another example of a time-symmetry breaking scenario which involves the admixture of a d_{xy} wave component [26,27] we refer to Ref. [5].

4. DPE from superconducting rings pierced by a magnetic flux

To inspect the influence of topology, we study the case of an isolated, phase-coherent, one-channel (1D) ring. The basic parameters are then the ring circumference L and the number of electrons N in the ring. Furthermore, we assume that $L\gg\xi_0$ and $\Delta>\delta$, where ξ_0 is the coherence length and $\delta=h^2N/(4\,\mathrm{mL}^2)$ is the level spacing at E_F. We consider an Aharonov–Bohm configuration, i.e., the ring is pierced by a magnetic flux $\Phi=\oint\mathbf{A}\cdot\mathrm{d}\mathbf{l}$, where $\mathbf{A}$ is the vector potential. The magnetic field $\mathbf{H}=\nabla\times\mathbf{A}$ is zero within the ring. The magnetic flux is measured in terms of the superconducting flux quantum $\Phi_s=\Phi_0/2$, with $\Phi_0\equiv hc/e$ being the usual flux quantum.

The wave numbers are then quantized such that $k\equiv(\pi n_k/L,\sigma)$ and n_k is the magnetic number which assumes integer values such that $n_k+n_q=$ even. $n_q=0,\pm1,\pm2,\ldots$ is the quantum number for the collective drift motion characterized by the wave vector

$$q=\frac{\pi}{L}\left(n_q+\frac{\Phi}{\Phi_s}\right). \tag{8}$$

The bogolon energies become

$$E_{k,q}=\frac{\hbar^2kq}{m}+\sqrt{\varepsilon^2_{k,q}+\Delta^2}\quad\text{where}$$
$$\left[\varepsilon_{k,q}=\frac{\hbar^2(k^2+q^2)}{2m}-E_F\right].$$

The coherence factors take on the form

$$u_k^2+v_k^2=1,\quad u_kv_k=\frac{\Delta}{2\sqrt{\varepsilon^2_{k,q}+\Delta^2}},$$

$$v_k^2=\frac{1}{2}\left(1-\frac{\varepsilon_{k,q}}{\sqrt{\varepsilon^2_{k,q}+\Delta^2}}\right).$$

The hole–hole spectral function acquires the form

$$A_{12}^{(-)}(k_1k_2k_1'k_2';E_{12})=(\delta_{k_1k_1'}\delta_{k_2k_2'}-\delta_{k_1k_2'}\delta_{k_2k_1'})\int\mathrm{d}E\,A_{k_1}^{(-)}(E)$$
$$\times A_{k_2}^{(-)}(E_{12}-E)+\delta_{k_1,-k_2}\delta_{k_1',-k_2'}u_{k_1}v_{k_1}u_{k_1'}v_{k_1'}$$
$$\times(1-f_{k_1,q}-f_{-k_1,q})(1-f_{k_1',q}-f_{-k_1',q})\delta(E_{12}).$$

The BCS one-hole spectral function is

$$A_k^{(-)}(E)=f_{k,q}u_k^2\delta(E-E_{k,q})+(1-f_{-k,q})v_k^2\delta(E+E_{-k,q}).$$

$f_{k,q}=1/[1+\exp(E_{k,q}/k_BT)]$ is the Fermi distribution function. The DPE current for this case is then given by

$$J_{12}\propto\sum_{k_1k_2}[|M_{k_1k_2}|^2-\mathrm{Re}(M_{k_1k_2}M^*_{k_2k_1})]\int\mathrm{d}E\,A_{k_1}^{(-)}(E)A_{k_2}^{(-)}$$
$$\times(E_{12}-E)+\delta(E_{12})\left|\sum_kM_{k,-k}u_kv_k(1-f_{k,q}-f_{-k,q})\right|^2. \tag{9}$$

The DPE matrix elements are smooth on the scale of several Δ's around $E_{12} = 0$ and hence

$$J_{12} = J_{\mathrm{UP}} + J_{\mathrm{CP}}, \quad J_{\mathrm{UP}} \propto \int \mathrm{d}E\, \mathcal{N}(E)\mathcal{N}(E_{12} - E),$$

$$J_{\mathrm{CP}} \propto \left|\frac{\Delta}{V}\right|^2 \delta(E_{12}).$$

$\mathcal{N}(E)$ is the density of occupied one-electron states and V is the matrix element of the pairing potential. As inferred from the above equation, the value of the gap Δ and hence the intensity of the CP component J_{CP} depend on both the temperature and the magnetic flux. If the magnetic flux exceeds the value $\Phi_d = (m\Delta L/\pi k_{\mathrm{F}}).\Phi_{\mathrm{s}}$ a depairing may occur for a very thin ring (a type II material). Clearly, in this specific regime the CP component vanishes and accordingly the DPE spectrum exhibits no peak at $E_{12} = 0$.

5. Conclusions

In summary, we outlined the potential of double photoemission for the study of the mechanisms of superconductivity. Examples for conventional and high- T_{c} materials have been discussed as well as finite size effects and the influence of an external magnetic flux.

References

[1] L.D. Landau, Zh. Eksp. Teor. Fiz. 30 (1956) 1058 (Sov. Phys.-JETP 3 (1957) 920); G.D. Mahan, Many Particle Physics, second ed., Plenum, New York, 1990.

[2] M. Tinkham, Introduction to Superconductivity, second ed., McGraw-Hill, Singapore, 1996.

[3] M. Sigrist, K. Ueda, Rev. Mod. Phys. 63 (1991) 239; A.P. Mackenzie, Y. Maeno, Rev. Mod. Phys. 75 (2003) 657.

[4] K.A. Kouzakov, J. Berakdar, Phys. Rev. Lett. 91 (2003) 257007.

[5] K.A. Kouzakov, J. Berakdar, Philos. Mag. 86 (2006) 2623.

[6] J. Berakdar, N.M. Kabachnik, Europhys. Lett. 70 (2005) 81.

[7] J. Bardeen, et al., Phys. Rev. 106 (1957) 162; J. Bardeen, et al., Phys. Rev. 108 (1957) 1175.

[8] L.N. Cooper, Phys. Rev. 104 (1956) 1189.

[9] J.R. Schrieffer, Theory of Superconductivity, W.A. Benjamin, Reading, MA, 1964; A.A. Abrikosov, et al., Methods of Quantum Field Theory in Statistical Physics, Dover, New York, 1975.

[10] J.G. Bednorz, K.A. Müller, Z. Phys. B 64 (1986) 189.

[11] E. Dagotto, Rev. Mod. Phys. 66 (1994) 763.

[12] D.J. Van Harlingen, Rev. Mod. Phys. 67 (1995) 515; J.R. Schrieffer, M. Tinkham, Rev. Mod. Phys. 71 (1999) S313; H. Matsui, et al., Phys. Rev. Lett. 90 (2003) 217002-1.

[13] A. Kaminski, et al., Nature 416 (2002) 610; C.M. Varma, Phys. Rev. B 61 (2000) R3804.

[14] S.B. Dierker, et al., Phys. Rev. Lett. 50 (1983) 853.

[15] R. Hackl, et al., J. Phys. Condens. Matter 16 (1983) 1792.

[16] B. Schrader (Ed.), Infrared and Raman Spectroscopy: Methods and Applications, VCH, Weinheim, 1995.

[17] T.J.B. Janssen, et al., Phys. Rev. B 57 (1998) 11698.

[18] M.D. Upward, et al., Phys. Rev. B 65 (2002) 220512-1.

[19] J. Schumann, Phys. Status Solidi B 99 (1980) 79.

[20] K.E. Kihlstrom, Phys. Rev. B 32 (1985) 2891.

[21] Z. Shen, D.S. Dessau, Phys. Rep. 253 (1995) 1.

[22] F. Reinert, et al., Phys. Rev. Lett. 85 (2000) 3930; A. Chainani, et al., Phys. Rev. Lett. 82 (2000) 1966; H. Uchiyama, et al., Phys. Rev. Lett. 88 (2002) 157002.

[23] D.J. Van Harlingen, Rev. Mod. Phys. 67 (1997) 515.

[24] A.A. Kordyuk, S.V. Borisenko, M. Knupfer, J. Fink, Phys. Rev. B 67 (2003) 064504.

[25] J.Y.T. Wei, N.-C. Yeh, W.D. Si, X.X. Xi, Physica B 284–288 (2000) 973.

[26] T.-K. Ng, C.M. Varma, Phys. Rev. B 70 (2004) 054514.

[27] R.B. Laughlin, Phys. Rev. Lett. 80 (1998) 5188.