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Particle–hole asymmetry in the scanning tunneling spectroscopy of the high temperature superconductors

Anna Gorczyca[1], **Mariusz Krawiec**[2], **Maciej M. Maśka**[1], and **Marcin Mierzejewski**[*, 1]

[1] Department of Theoretical Physics, Institute of Physics, University of Silesia, 40-007 Katowice, Poland
[2] Institute of Physics and Nanotechnology Center, M. Curie-Sklodowska University, Pl. M. Curie-Sklodowskiej 1, 20-031 Lublin, Poland

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There is still no consensus on the mechanism that is responsible for a particle–hole asymmetry observed in scanning tunneling spectroscopy of high-temperature superconductors. According to the most popular hypothesis this asymmetry results from strong Coulomb correlations in a nearly half-filled band. In the present paper we propose another mechanism that leads to such asymmetry. It originates from the coupling between the superconductor and the substrate that the system is deposed on. We show that this coupling gives rise to the particle–hole asymmetry only in the case of an anisotropic superconductivity.

1 Introduction

The scanning tunneling microscopy (STM) is a powerful real space technique which is very sensitive to local atomic and electronic structures [1, 2]. It allows one to study the properties of various, not necessarily periodic, structures with atomic resolution. Since the invention of STM [3], it has widely been applied to analyze surface reconstructions [2], low dimensional structures [1, 2, 4–6], and high-temperature superconductors [7]. While the STM is usually used to characterize topography of various structures, it is also suitable to study the electronic structure, measuring current–voltage characteristics. With this technique, known as a scanning tunneling spectroscopy (STS), one can perform spectroscopic measurements with a spatial resolution down to the atomic scale. Thus STS is a complementary technique to others, like angle resolved photoemission (ARPES) or optical spectroscopy operating in k-space. The STS allows one to measure local density of states not only below the Fermi energy (like ARPES) but also above it. Depending on applied tip-substrate voltage, one can get information on occupied and empty electron states of the structure with high spatial and energy resolution.

STM has recently played an important role also in understanding of the strongly correlated systems, especially high temperature superconductors. In particular, the local density of states, obtained in the STS experiments, provides crucial information concerning the vortex structure [8] and nanoscale inhomogeneity of the superconducting gap in the absence of external magnetic field [9]. One of the most striking results concerns a strong asymmetry between the spectral weights obtained for positive and negative bias [10]. This asymmetry does not occur in conventional superconductors [11]. It is particularly visible in the height of coherence peaks for occupied and unoccupied states. The commonly accepted explanation has been suggested by Anderson. Since there is only a small number of holes in the lower Hubbard subband and strong Coulomb repulsion results in a large energy gap between the lower

[*] Corresponding author: e-mail: marcin@phys.us.edu.pl

and upper subbands, it is much easier to remove and electron than to add one. This idea has further been developed by Randeria et al. in Ref. [12].

In the STM experiments, the investigated system is coupled to two electrodes: STM tip and the substrate that the system is deposed on. Additionally, the flow of the current indicates that one deals with a system in a nonequilibrium state. The coupling between the system under investigation and the electrodes may lead to substantial modifications of its properties [13]. In the present paper, we calculate the STM current through the superconducting plane with the help of a formalism developed for nonequilibrium systems, namely, the Keldysh Green functions. We demonstrate that the coupling between the superconducting plane and the substrate itself leads to a particle–hole asymmetry in the current–voltage characteristics. This asymmetry may contribute to the asymmetry, that originates from the presence of strong electronic correlations.

2 Model and results

In the following we investigate a superconducting plane coupled to two electrodes: the STM tip and the substrate. The Hamiltonian under consideration is assumed to be of the form

$$\mathcal{H} = \mathcal{H}_{\mathrm{SC}} + \mathcal{H}_{\mathrm{SC-EL}} + \mathcal{H}_{\mathrm{EL}} \,. \tag{1}$$

The first term in Eq. (1) describes the investigated superconducting system

$$\mathcal{H}_{\mathrm{SC}} = -\sum_{l,m,\sigma} t_{lm} c^{\dagger}_{l\sigma} c_{m\sigma} + \sum_{j,\sigma} \tilde{\varepsilon}_j c^{\dagger}_{j\sigma} c_{j\sigma} + \sum_{l,m} (\Delta_{lm} c^{\dagger}_{l\uparrow} c^{\dagger}_{m\downarrow} + \Delta^{*}_{lm} c_{l\downarrow} c_{m\uparrow}) \,, \tag{2}$$

where $c_{l\sigma}$ annihilates and electron with spin σ at site l, t_{lm} is the hopping integral and Δ_{lm} stands for the superconducting order parameter. $\tilde{\varepsilon}_j = \varepsilon_j - \mu$, where ε_j is the atomic energy at site j and μ is the chemical potential. The coupling between the superconducting plane and the electrodes consists of two terms:

$$\mathcal{H}_{\mathrm{SC-EL}} = \sum_{\boldsymbol{k}\in \mathrm{sub},l,\sigma} V^{s}_{l\boldsymbol{k}} (c^{\dagger}_{s\boldsymbol{k}\sigma} c_{l\sigma} + \mathrm{h.c.}) + \sum_{\boldsymbol{k}\in \mathrm{tip},\sigma} (V^{t}_{\boldsymbol{k}} c^{\dagger}_{i\sigma} c_{t\boldsymbol{k}\sigma} + \mathrm{h.c.}) \,. \tag{3}$$

Here $c^{\dagger}_{s\boldsymbol{k}\sigma}$ creates an electron with momentum $\boldsymbol{k}$ in the substrate, whereas $c^{\dagger}_{t\boldsymbol{k}\sigma}$ is the creation operator for an electron in the STM tip. In Eq. (3) we have distinguished site i of the superconducting plane, that is just below the STM tip. We assume that both the electrodes can be described as noninteracting systems:

$$\mathcal{H}_{\mathrm{EL}} = \sum_{\boldsymbol{k}\in \mathrm{sub},\sigma} \varepsilon_{s\boldsymbol{k}} c^{\dagger}_{s\boldsymbol{k}\sigma} c_{s\boldsymbol{k}\sigma} + \sum_{\boldsymbol{k}\in \mathrm{tip},\sigma} \varepsilon_{t\boldsymbol{k}} c^{\dagger}_{t\boldsymbol{k}\sigma} c_{t\boldsymbol{k}\sigma} \,. \tag{4}$$

Figure 1 shows a schematic view of the system under consideration.

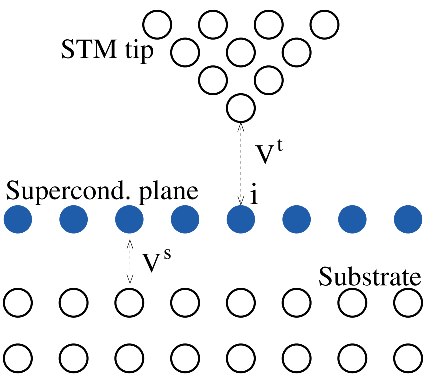

Fig. 1 (online colour at: www.pss-b.com) Schematic plot of the investigated STM system.

In order to determine the current flowing through the superconducting plane we follow standard derivation [14] and get

$$J = \frac{e}{h} \int_{-\infty}^{\infty} \mathrm{d}\omega\, T(\omega)\, [f^s(\omega) - f^t(\omega)]\,, \tag{5}$$

where f^s and f^t are the Fermi distribution functions of the substrate and STM tip, respectively, whereas the transmittance is given by:

$$T(\omega) = 2\Gamma^t \sum_{k,l} G^r_{ik}(\omega)\, \Gamma^s_{kl} G^a_{li}(\omega)\,. \tag{6}$$

The parameter $\Gamma^t(\omega) = \sum_{\boldsymbol{k}} |V^t_{\boldsymbol{k}}|^2\, \delta(\omega - \varepsilon_{t\boldsymbol{k}})$ denotes strength of the coupling between the tip atom and STM electrode, while $\Gamma^s_{kl}(\omega) = \sum_{\boldsymbol{k}} |V^s|^2\, \mathrm{e}^{i\boldsymbol{k}(\boldsymbol{R}_k - \boldsymbol{R}_l)}\, \delta(\omega - \varepsilon_{s\boldsymbol{k}})$ is the coupling between superconducting plane atoms at positions $\boldsymbol{R}_k$ and $\boldsymbol{R}_l$ via the substrate. In other words, it describes hopping of the electron from site k to site l through the substrate states [15]. In the following we have neglected the energy dependence of the matrices Γ and assumed constant energy bands in the electrodes. Thus the coupling between superconducting plane and the substrate can be expressed in the form [15]

$$\Gamma^s_{kl} = \Gamma^s\, \frac{\sin\,(k_{\mathrm{F}} a R_{kl})}{k_{\mathrm{F}} a R_{kl}}\,, \tag{7}$$

where k_{F} is the Fermi wave vector of the substrate electrode, and R_{kl} is the distance between sites k and l measured in units of the lattice constant a. In typical metals $k_{\mathrm{F}}a$ is of the order of 4–5.

The transmittance $T(\omega)$ (Eq. (6)), and thus current J (Eq. (5)), depends on the retarded and advanced Green functions, as obtained from the solution of the equation

$$\sum_{j'} \hat{A}_{mj'} \hat{G}^{r(a)}_{j'j} = \delta_{mj}\, \tau_0\,, \tag{8}$$

where

$$\hat{A}_{mj'} = \tau_0 \omega \delta_{mj'} - (\Delta_{mj'}\tau^+ + \Delta^*_{mj'}\tau^- - t_{mj'}\tau_3 + \tilde{\varepsilon}_m \delta_{mj'}\tau_3) + \frac{i}{2}\, \tau_0 [\Gamma^t(\omega)\, \delta_{mi}\delta_{j'i} + \Gamma^s_{mj'}(\omega)]\,, \tag{9}$$

and $\hat{G}^{r(a)}_{j'j}$ in the Nambu notation has the following form:

$$\hat{G}^{r(a)}_{j'j} = \begin{bmatrix} \langle\langle c_{j'\uparrow} | c^\dagger_{j\uparrow} \rangle\rangle & \langle\langle c_{j'\uparrow} | c_{j\downarrow} \rangle\rangle \\ \langle\langle c^\dagger_{j'\downarrow} | c^\dagger_{j\uparrow} \rangle\rangle & \langle\langle c^\dagger_{j'\downarrow} | c_{j\downarrow} \rangle\rangle \end{bmatrix}. \tag{10}$$

In Eq. (9) τ_i represent the Pauli matrices for $i = 1, 2, 3$, and $\tau^{\pm} = 1/2(\tau_1 \pm i\tau_2)$.

3 Discussion and remarks

We have calculated the current–voltage characteristic of the superconducting plane and the local density of states (LDOS). We have considered two cases: (i) s-wave pairing with the superconducting order parameter $\Delta_{lj} = \Delta_s \delta_{lj}$ and (ii) d-wave pairing with $\Delta_{lj} = \pm\, \Delta_d \delta'_{\langle lj \rangle}$, where $\delta'_{\langle lj \rangle} = 1$ for neighboring sites l, j and 0 otherwise. We have considered only the nearest-neighbor hopping $t_{lj} = t\delta'_{\langle lj \rangle}$. Then, the particle-hole symmetry is present for the half-filled case $\tilde{\varepsilon}_j = 0$, provided the system is disconnected from the STM tip and the substrate. Therefore, occurrence of any asymmetry has to be attributed to this coupling.

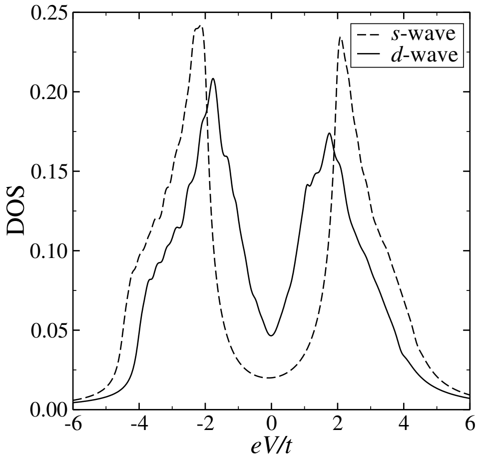

Fig. 2 Local density of states for a 26×24 cluster obtained for $\Gamma^s = 0.8t$ and $\Gamma^t = 0.02t$. The superconducting order parameter for the case of s-wave pairing is $\Delta_s = 2t$ and for d-wave pairing $\Delta_d = 0.5t$ $(t > 0)$. The value of the Fermi wave vector is $k_F a = 4$.

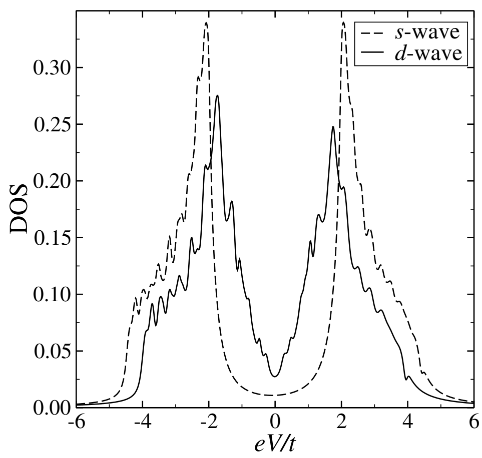

Fig. 3 Local density of states for a 26×24 cluster obtained for $\Gamma^s = 0.4t$. Other parameters are the same as in Fig. 2.

In order to mimic the experimental situation we have assumed that the coupling between the superconducting plane and the substrate is much larger that its coupling to the STM tip: $\Gamma^s \gg \Gamma^t$.

As expected, LDOS is found to be proportional to the differential conductance dI/dV. Therefore we restrict the presentation of our numerical results only to LDOS, calculated from the retarded Green functions.

We have calculated LDOS for a 26 × 24 cluster with periodic boundary conditions (bc). In order to avoid unphysical degeneracy of states at the Fermi level, which occurs for the half-filled band in calculations on square clusters with fixed or periodic bc taken in both directions [16], we have chosen different number of lattice sites along x- and y-axes.

In Figs. 2 and 3 we compare LDOS for s- and d-wave superconductivity for a moderate and strong coupling Γ^s between the superconducting plane and the substrate. One can see a strong asymmetry of

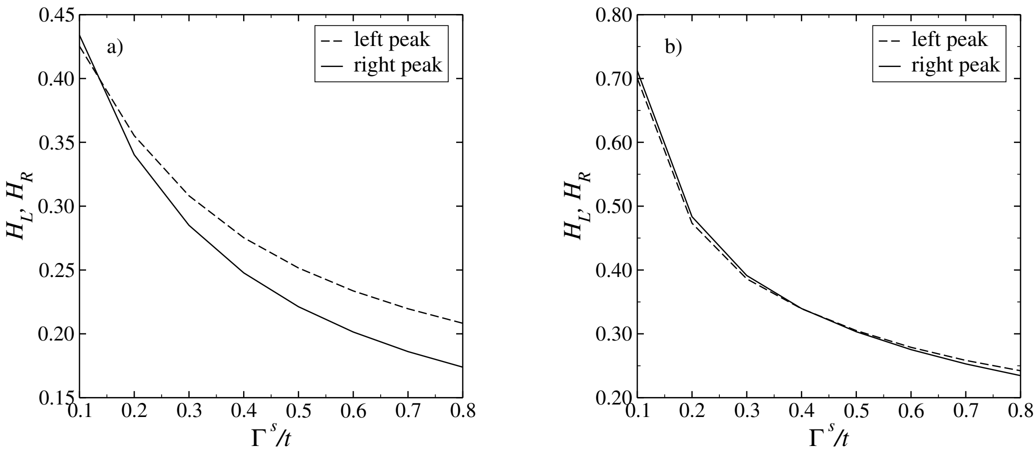

Fig. 4 Heights of the coherence peaks in LDOS as a function of Γ^s for d-wave (a) and s-wave (b) pairing. The model parameters are the same as in Fig. 2.

the height of the coherence peaks in the case of d-wave pairing. Generally, this asymmetry could originate from the coupling between the superconducting system and both the electrodes. However, since the coupling to the STM tip is many order of magnitude smaller than the coupling to the substrate, the latter interaction should be the crucial one. Comparison of Figs. 2 and 3 indicates that the asymmetry increases with increasing coupling between the system and the substrate, what confirms this assumption. Figure 4 explicitly illustrates this dependence.

Two questions arise: why the coupling to the substrate gives rise to the particle–hole asymmetry and why the peak at negative bias is higher than the peak at the positive one. As to the first question, one can note that the coupling to the electrodes enables the charge carriers to move between lattice sites through the substrate. Therefore, this coupling can affect the system in an analogous way as the next nearest neighbor hopping integrals do, resulting in an asymmetric density of states. Concerning the second question, it is easy to show that the density of states $\rho(\omega)$ changes to $\rho(-\omega)$ upon the inversion of the sign of the hopping integral t.

It is interesting that this asymmetry does not occur for isotropic s-wave superconductivity. Additionally, we have found that the degree of the asymmetry increases with the magnitude of the superconducting gap. Both these features explain why the discussed asymmetry is not observed in conventional superconductors.

To conclude, we have proposed a new mechanism leading to the particle–hole asymmetry. Similar asymmetry has recently been observed in the STM experiments on the high-temperature superconductors. The asymmetry discussed in the present paper originates from the coupling between the superconducting system and the electrodes. It should be visible in superconducting systems with a large anisotropic gap. Probably, this effect alone is insufficient to explain the experimental results, however, it can cooperate with other possible mechanisms leading to such an asymmetry, e.g., with strong Coulomb repulsion. Therefore, it would be interesting to take both these effects simultaneously into account.

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