Analyzing scanning tunneling spectroscopy for Fe-based superconductors and extracting sample density of states

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Abstract

We extract the density of states (DOS) from the scanning tunneling spectroscopy data for Ba$_{1-x}$K$_x$Fe$_2$As$_2$ superconductor. The obtained sample DOS is composed of two ordinary s-wave types from the band at Γ point and a linear-like DOS within the s-wave gap from the band at M point in the Brillouin zone, and is consistent with the corresponding data from angle-resolved photoemission spectroscopy. We clarify that the major peak of the tunneling conductance is not related to the DOS but is rather the effect of nonequilibrium coherent tunneling including all coherent spins in the tip and sample.

Keywords: iron-based superconductors, scanning tunneling spectroscopy, sample density of states

(Some figures may appear in colour only in the online journal)

1. Introduction

The high transition temperature observed in single-layer FeSe on SrTiO$_3$ (FeSe/STO) [1, 2] discovered recently has further heightened interest in Fe-based superconductors. These superconductors have multiple Fermi surfaces around Γ and M points in the Brillouin zone [3], even though the band at the Γ point is largely suppressed below the Fermi level in single-layer FeSe/STO [4, 5]. Such multiplicity of Fermi surfaces raises a big challenge not only to identify the sample density of states (DOS) but also to explain the tunneling conductance line shape as measured by scanning tunneling spectroscopy (STS) [6, 7].

Fundamental information on exotic superconductors is usually obtained by two spectroscopic tools, namely angle-resolved photoemission spectroscopy (ARPES) and STS. But a clearly known fact is that the proposed superconducting gaps by ARPES and STS differ on a meaningful scale; this is a long-standing puzzle in studying both cuprate [8–10] and Fe-based superconductors [6, 7, 11]. Another aspect of the Fe-based superconductor is the non-observation of s-wave DOS in the tunneling conductance [6, 7], even though the material has been claimed to be an s$^{\pm}$-wave superconductor [12]. These two particular aspects—the inconsistency between ARPES and STS and the lack of s-wave DOS in the tunneling conductance—are important issues which must be clarified.

Since a photon does not experience Coulomb interaction in a collision with correlated material, we expect that the ARPES setup does not encounter any theoretical difficulty in explaining its output. However, when an electron enters a correlated sample, strong Coulomb repulsion plays a crucial role in the subsequent tunneling dynamics. The STS setup sketched in figure 1(a) therefore requires a sophisticated theoretical treatment because the coherent tunneling here occurs in a many-body entangled state involving all coherent spins in the tip and sample. The purpose of this study is to solve the two problems mentioned above by explicitly obtaining the sample DOS from existing STS data and analyzing the contributions from different Fermi surfaces.

Among the many Fe-based superconductors, we focus on Ba$_{1-x}$K$_x$Fe$_2$As$_2$ [6] and single-layer FeSe/STO [2], because the former has contributions from bands at both Γ and M points while the latter is known to have contributions mostly from a band at the M point [4, 5]. Therefore, a comparative
analysis of the STS data of these two materials will be helpful to understand the nature of Fe-based superconductors.

The prevailing interpretation of tunneling conductance, which is believed as the sample DOS, is valid for materials without correlation effects. However, when tunneling occurs in a correlated material with a bias weaker than on-site Coulomb repulsion, an electron cannot simply hop to the mediating site (MS) under the tip if an electron already occupies the MS. In such a case, the only possible way for a coherent current to flow is to form a linearly combined singlet connecting the tip and sample, as shown in figure 1(a), and perform a process of singlet co-tunneling, changing singlet partner, and then co-tunneling again, repeatedly. In this circumstance, the entering electron does not feel strong Coulomb repulsion at the MS. Here, all coherent spins in the tip and all Cooper pairs in the sample are involved in coherent tunneling by the linearly combined two singlets connecting the tip, MS, and sample; we call this entangled state tunneling. Many incoherent spins also exist in the STS system, and even though they do not join in coherent current they influence current flow by causing double occupancy at the MS. Accordingly, the effects of both coherent and incoherent spins should be properly treated in related tunneling theory.

Various theoretical techniques handling two-reservoir Kondo or Anderson impurity model under bias, which is similar to figure 1(b) with constant sample DOS, have been reported. These techniques include real-time renormalization group method [13], Keldysh formalism [14], quantum Monte Carlo calculations [15], dynamical Bethe ansatz [16], and scattering state renormalization group approach [17]. However, these techniques have not been extended to the case for correlated superconductors on which we are focusing in this study.

This study is designed as follows. We introduce a tunneling conductance formula and the Green’s function technique in Liouville space in order to construct a simplified theoretical conductance formula and the Green’s function at the MS under the tip if an electron already occupies the MS. In such a case, the only possible way for a coherent current to flow is to form a linearly combined singlet connecting the tip and sample, as shown in figure 1(a), and perform a process of singlet co-tunneling, changing singlet partner, and then co-tunneling again, repeatedly. In this circumstance, the entering electron does not feel strong Coulomb repulsion at the MS. Here, all coherent spins in the tip and all Cooper pairs in the sample are involved in coherent tunneling by the linearly combined two singlets connecting the tip, MS, and sample; we call this entangled state tunneling. Many incoherent spins also exist in the STS system, and even though they do not join in coherent current they influence current flow by causing double occupancy at the MS. Accordingly, the effects of both coherent and incoherent spins should be properly treated in related tunneling theory.

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This study is designed as follows. We introduce a tunneling conductance formula and the Green’s function technique in Liouville space in order to construct a simplified theoretical model appropriate to describe the STS system under consideration in section 2. In section 3, we determine the basis operators spanning the working Liouville space, and present an explicit expression of nonequilibrium expectation for the entangled state tunneling under consideration. Then, we prove the orthogonality of the basis operators. In section 4, we obtain a Liouville matrix and express the tunneling conductance as a function of sample DOS. We present the results of fitting an experimental tunneling conductance of single-layer FeSe/STO [2] and Ba1−xKxFexAs2 [6] with our extracted sample DOS in section 5, where we explicitly show that the sample DOS is indeed composed of ordinary s-wave DOS coming from the band at the Γ point and a linear-type DOS from the band at the M point. Our work concludes with discussion in section 6.

2. Green’s function via Liouville approach

We employ a tunneling conductance formula derived from the Meir–Wingreen current formula [18].

\[
\frac{dI}{dV} = \frac{e^2}{\hbar} \tilde{\Gamma}(\omega) \rho_d(\omega) \bigg|_{\omega=eV},
\]

where \( I \) and \( V \) are current and bias voltage between tip and sample, \( \Gamma(\omega) = \Gamma^T(\omega)\Gamma^S(\omega)/[\Gamma^T + \Gamma^S(\omega)] \) is the effective coupling of the tip, MS, and sample, and \( \Gamma^S(\omega) = 2\pi(\hbar V)^2 D(\omega) \), where \( D(\omega) \) denotes the sample DOS. In the entangled state tunneling, entanglement is formed by two singlet states sketched in figure 1 and tunneling current is given by sum of individual entanglement represented by \( \omega_i \). Then, the proportionality condition, \( \Gamma^T(\omega_i, \pm eV) \propto \Gamma^S(\omega_i) \), is satisfied, and equation (1) becomes valid with bias-independent local DOS \( \rho_d(\omega) \) that is different from the sample DOS \( D(\omega) \). We consider that \( \rho_d(\omega) \) is bias-independent when the tip and sample are entangled, as shown in figure 1.

The key quantity of equation (1) is the local DOS at the MS, which is given by the Green’s function at the MS:

\[
\rho_d(\omega) = -\frac{1}{\pi} \text{Im} \tilde{G}_{dd}^+(\omega). \]

This Green’s function \( \tilde{G}_{dd}^+(\omega) \) should not be obtained at equilibrium but rather at steady-state nonequilibrium. We employ the resolvent Green’s function in the operator space, called the Liouville space [19],

\[
\tilde{G}_{pq}^+(\omega) = \langle \hat{e}_p | (\omega + i\delta)I - \hat{L} \rangle^{-1} |\hat{e}_q\rangle,
\]

where \( \hat{e}_p \) is the basis operator of the Liouville space, \( I \) is the identity operator, and \( \hat{L} \) is the Liouville operator defined by \( \hat{L} \hat{O} = \hat{H}O - O\hat{H} \) for operator \( \hat{O} \). The inner product in the Liouville space is defined by \( \langle A|B \rangle \equiv \langle AB^\dagger + B^\dagger A \rangle \), where \( B^\dagger \) is the adjoint of \( B \) and the angular brackets denote the expectation value at steady-state nonequilibrium. Equation (2) is a generic form of Green’s function along with one using a Hamiltonian. The reason we employ the Liouville approach instead of the well-known Hamiltonian approach is the availability of basis operators [19–21]; the basis state vectors spanning the Hilbert space of a correlated system are not easily obtained.

The STS setup of figure 1(a) is described by the theoretical model.
Liouville matrix

\[ H = \sum_{p,\sigma} E_p c_{p\sigma}^T c_{p\sigma} + V_T \sum_{p,\sigma} (c_{p\uparrow}^T d_{\sigma} + d_{\sigma}^T c_{p\uparrow}) + U n_d n_{\bar{d}} + \sum_{k,\sigma} E_k c_{k\sigma}^T c_{k\sigma}^T + \sum_{k,k'} M_{kk'} c_{k\sigma}^T c_{k'\sigma}^T + V_T \sum_{p,\sigma} (c_{p\uparrow}^T d_{\sigma} + d_{\sigma}^T c_{p\uparrow}) + U n_d n_{\bar{d}} \]

where the superscripts \( T \) and \( S \) denote the tip and superconductor sample, respectively. We perform the Bogoliubov transformation for the fermion operators of superconductors using \( c_{k\sigma}^T = u_{k} \alpha_{k\sigma}^T + v_k \alpha_{-k\bar{\sigma}} \) and \( c_{-k\bar{\sigma}}^T = u_k \alpha_{-k\bar{\sigma}} - v_k \alpha_{k\sigma} \). Then, the second line of equation (3) changes to \( E_0 + \sum_k E_k (\alpha_{k\uparrow}^T \alpha_{k\uparrow} + \alpha_{-k\bar{\sigma}}^T \alpha_{-k\bar{\sigma}}) \) by neglecting quasiparticle interaction, which is valid at zero temperature, where \( E_0 \) is the ground state energy of the superconductor and \( E_k \) is the excitation energy of the Bogoliubov quasiparticles. Here, \( E_0 \) and \( E_k \) are written as \( E_0 = 2 \sum_k \varepsilon_k v_k^2 - \sum_k v_k^2 |M_{kk'} | u_k v_k u_{k'} v_{k'} \) and \( E_k = \varepsilon_k (u_k^2 - v_k^2) + 2 \sum_k |M_{kk'} | u_k v_k u_{k'} v_{k'} \). Then, the Hamiltonian of equation (3) is transformed into a two-reservoir quantum impurity system, as

\[ H = \sum_{p,\sigma} E_p c_{p\sigma}^T c_{p\sigma} + V_T \sum_{p,\sigma} (c_{p\uparrow}^T d_{\sigma} + d_{\sigma}^T c_{p\uparrow}) + U n_d n_{\bar{d}} \]

which is depicted in figure 1(b). This system has a flat DOS for the tip and a DOS given by \( D(\omega) = \sum_k \delta(\omega - E_k) \) for the sample. Our main purpose is to find \( D(\omega) \) from tunneling data.

To calculate the Green’s function of equation (2), the first step is to determine the complete set of basis operators. One advantage of using the Liouville approach is that, as shown with different colors in figure 2, the basis operators are clearly classified into three subgroups that play distinct roles: the reservoir (light green), the MS (yellow), and hybridization (light blue). Then, the Liouville matrix has an important section representing tip-sample coherence at both corners of the matrix, as shown by the orange regions in figure 2.

For up-spin dynamics \( d_1(t) \), the MS is described by \( d_2 \) solely due to strong on-site Coulomb repulsion at the MS, and the reservoir is described by \( c_{k\uparrow}^T \) where \( k = 1, 2, \cdots, \infty \). A nontrivial part of the basis operators is that describing hybridization, which also has infinite degrees of freedom. Fortunately though, the property of unidirectional movement in entangled state tunneling restricts multiple back-and-forth processes, and this greatly simplifies the degrees of freedom for hybridization. Thus, the Liouville matrix has infinite-dimensional parts only in the sectors describing the non-interacting reservoirs, as shown by the light green regions in figure 2. Since these non-interacting reservoirs (tip and sample) are represented by diagonal blocks, the Liouville matrix can be reduced to a finite-dimensional matrix (indicated by the dashed line in figure 2) by way of a matrix reduction scheme [20, 22, 23]. Such matrix reduction corresponds to tracing out the degrees of freedom of the non-interacting reservoirs.

3. Orthonormal basis operators and Nonequilibrium expectation

Specifically for \( d_1(t) \) dynamics, the MS is described by \( d_2 \) only, the tip (sample) is described by \( c_{k\uparrow}^T (\alpha_{k\uparrow}) \) and \( n_{d\downarrow} c_{k\downarrow}^T (n_{d\downarrow} \alpha_{k\downarrow}) \).
where \( k = 1, 2, \cdots, \infty \), and the hybridization is described by \( \tilde{J}_{\uparrow \downarrow}^{k} = \tilde{V} \sum_{c_{k}^{\uparrow}, c_{k}^{\downarrow}} (c_{k}^{\uparrow} d_{k} + d_{k}^{\dagger} c_{k}^{\downarrow}) \) and \( \tilde{J}_{\uparrow \uparrow}^{k} = \tilde{V} \sum_{c_{k}^{\uparrow}, c_{k}^{\downarrow}} (c_{k}^{\uparrow} d_{k}^{\dagger} - d_{k}^{\dagger} c_{k}^{\downarrow}) \). The working Liouville space for the entangled state tunneling in STS is spanned by the following basis operators divided into three groups:

\[
\begin{align*}
\{ c_{k}^{\uparrow}, c_{k}^{\downarrow} & \alpha n_{d_{k}} / (\langle \alpha n_{d_{k}} \rangle)^{1/2}, \quad k = 0, 1, \ldots, \infty; \\
\{ d_{k}^{\dagger} d_{k}^{\dagger} & \alpha \delta n_{d_{k}} / (\langle \alpha \delta n_{d_{k}} \rangle)^{1/2}, \quad k = 0, 1, \ldots, \infty; \\
\{ \alpha k \uparrow \delta n_{d_{k}} / (\langle \alpha k \delta n_{d_{k}} \rangle)^{1/2}, \quad k = 0, 1, \ldots, \infty,
\end{align*}
\]

where we introduced \( \delta \) indicating \( \delta O = O - \langle O \rangle \) to achieve orthogonality among the basis operators. We omit normalization factors \( (\langle \delta n_{d_{k}} \rangle)^{1/2} \) in the denominators of the corresponding basis operators in the second line. Orthogonality between an operator without \( \delta \) and one with \( \delta \) is obvious; however, proving orthogonality among operators containing \( \delta \) is nontrivial. Orthogonality for the latter case is clarified after determining the expectation scheme for entangled state tunneling at steady-state nonequilibrium below.

In STS of a correlated system in which both tip and sample are within the coherent region, tunneling must be entangled state tunneling, as depicted in figure 1(b). Under this circumstance, three different types of coherent processes as sketched in figure 3 are considered: (a) one comprising two singlet co-tunnelings, (b) one comprising two spin exchanges describing Kondo coupling, and (c) one comprising spin exchange and singlet co-tunneling. Figure 3(a) transports two electrons (red arrows) after one cycle, figure 3(b) represents Kondo coupling dynamics on the left side, and figure 3(c) transports one electron (red arrow) after one cycle. One cycle thus comprises four hybridization processes.

The steady-state nonequilibrium expectation for figure 3(a) is expressed by

\[
\langle \Psi_{0} | \tilde{V}^{\delta}_{\uparrow \downarrow} (c_{k}^{\uparrow} d_{k}^{\dagger} c_{k}^{\downarrow} d_{k}^{\dagger} c_{k}^{\downarrow}) d_{k} \rangle / \Delta_{0},
\]

while for figure 3(c) by

\[
\langle \Psi_{0} | \tilde{V}^{\delta}_{\uparrow \downarrow} (c_{k}^{\uparrow} d_{k}^{\dagger} c_{k}^{\downarrow} d_{k}^{\dagger} c_{k}^{\downarrow}) d_{k} \rangle / \Delta_{0},
\]

where \( |\Psi_{0}\rangle \) denotes the initial and final state wavefunction of figure 3 and \( \Delta_{0} \) is the energy unit. Then, the steady-state nonequilibrium expectation for electron transfer from the sample to tip should be written as \( \langle \Psi_{0} | \tilde{V}^{\delta}_{\uparrow \downarrow} (\text{operators}) d_{k} | \Psi_{0} \rangle / \Delta_{0} \). For the reverse movements of figures 3(a) and (c), i.e., transfer from the sample to tip, replacing sample operators by tip operators and vice versa along with changing the hybridization parameter is needed:

\[
\langle \Psi_{0} | \tilde{V}^{\delta}_{\uparrow \downarrow} (\alpha k \uparrow \delta n_{d_{k}} / (\langle \alpha k \delta n_{d_{k}} \rangle)^{1/2}, \quad k = 0, 1, \ldots, \infty)
\]

Thus, the steady-state nonequilibrium expectation for moving from the sample to tip is written as \( \langle \Psi_{0} | \tilde{V}^{\delta}_{\uparrow \downarrow} (\text{operators}) d_{k} | \Psi_{0} \rangle / \Delta_{0} \). These steady-state nonequilibrium expectations are bias-independent, which is consistent with the bias-independence of the local DOS mentioned in section 2. Expectation for six operators appear in the inner products among the basis operators including \( \alpha \). One can easily check the orthogonality among those basis operators by inner products among the basis operators including \( \alpha \).
4. Liouville matrix

The structure of Liouville matrix $\mathbf{L}$, sketched in figure 2 is composed of two diagonal blocks sharing the MS and the corner blocks. Each diagonal block comprises three parts: an $\infty \times \infty$ diagonal block for the non-interacting reservoir, a region of hybridization, and a region for the MS. The corner block contains a tip-sample coherent superposition indicated in orange and a null block indicated in white due to the lack of direct transition between the tip and sample. One can reduce the $\infty$-dimensional Liouville matrix to a finite-dimensional matrix because the tip and sample are represented by diagonal blocks [20, 22, 23]. Thus, the Liouville matrix is $\mathbf{L}_{a} = \mathbf{L}_{d} + \Sigma$, where $\mathbf{L}_{d}$ is given by

$$
\mathbf{iL}_{d} = \begin{pmatrix}
0 & \gamma^{T} & \gamma^{S}_{TS} & \gamma^{S}_{A} \\
-\gamma^{T} & 0 & \gamma^{S}_{TS} & \gamma^{S}_{A} \\
\gamma^{S}_{TS} & \gamma^{S}_{TS} & 0 & \gamma^{S} \\
\gamma^{S}_{A} & \gamma^{S}_{A} & -\gamma^{S} & 0 \\
\end{pmatrix},
$$

which is the central block indicated by the dashed line in figure 2, and $\Sigma$ denotes the self-energy matrix created in the process of matrix reduction, composed of the elements $\Sigma_{pq} = \beta_{pq} |\Gamma^{T} + 1^{\delta}(\omega)|/2$ with the coefficients $\beta_{pq}$ coming from the reduction process [20]. In the atomic limit, where the peaks are given by $\delta$ functions, the Coulomb peaks position at $\pm U/2$ with $\beta_{pq} = 0.25$ in a $T$-$S$ symmetric case except for $\beta_{33}$. Slight increases occur by correlations. Hence, we commonly choose $\beta_{11} = \beta_{15} = \beta_{33} = 0.252$, $\beta_{12} = \beta_{14} = 0.25 \beta_{22} = \beta_{24} = \beta_{44} = 0.25 \beta_{33} = 1$ and $\beta_{13} = \beta_{23} = \beta_{43} = \beta_{33} = 0$ in all strongly correlated systems [20, 24].

Each matrix element has its own role. The element $\gamma^{T(S)}$ is given by

$$
\gamma^{T(S)} = \frac{\sum_{k} i(\mathbf{V}^{T(S)} \tilde{\mathbf{c}}_{k}^{\dagger} + \mathbf{V}^{S} \alpha_{k})(\mathbf{d}^{T(S)} \mathbf{j}_{d}^{+} \mathbf{j}_{d}^{-})}{\langle (\delta_{d}^{T(S)})_{2} \rangle^{1/2} \langle (\delta_{d}^{T(S)})_{2} \rangle^{1/2}}.
$$

The first term of $\gamma^{T}$ describes figure 2(c) using $\langle \mathbf{j}_{d}^{+} \mathbf{j}_{d}^{-} \rangle = 2 i(\mathbf{V}^{T})^{T} \mathbf{c}_{k}^{\dagger} \mathbf{d}_{1} \mathbf{c}_{k} \mathbf{d}_{1}^{\dagger}$ and the expectation $\langle \mathbf{c}_{k}^{\dagger} \mathbf{V}^{S} \alpha_{k} \mathbf{c}_{k} \rangle$ (operators $\mathbf{d}_{1} \mathbf{c}_{k}^{\dagger}$). The second term describes moving in the reverse direction with spin exchange first using $\langle \mathbf{c}_{k}^{\dagger} \mathbf{V}^{T} \mathbf{c}_{k}^{\dagger} \rangle$ (operators) $\mathbf{d}_{1} \mathbf{c}_{k}^{\dagger}$, while the second term describes moving in the reverse direction with spin exchange first using $\langle \mathbf{c}_{k}^{\dagger} \mathbf{V}^{T} \mathbf{c}_{k}^{\dagger} \rangle$ (operators) $\mathbf{d}_{1} \mathbf{c}_{k}^{\dagger}$. On the other hand, figure 3(b), which describes Kondo coupling at equilibrium, is the case employing the first term of $\gamma^{T}$ using the expectation $\langle \mathbf{c}_{k}^{\dagger} \mathbf{V}^{T} \mathbf{c}_{k}^{\dagger} \rangle$ (operators) $\mathbf{d}_{1} \mathbf{c}_{k}^{\dagger}$. But this is not the dynamics of steady-state nonequilibrium because no electron transport occurs.

The elements $\gamma^{S}_{TS}$ are written as

$$
\gamma_{TS}^{S} = \frac{\sum_{k} i(\mathbf{V}^{T} \mathbf{c}_{k}^{\dagger} + \mathbf{V}^{S} \alpha_{k})(\mathbf{d}^{T(S)} \mathbf{j}_{d}^{+} \mathbf{j}_{d}^{-})}{\langle (\delta_{d}^{T(S)})_{2} \rangle^{1/2} \langle (\delta_{d}^{T(S)})_{2} \rangle^{1/2}},
$$

and

$$
\gamma_{A}^{TS} = \frac{(\sum_{k} i(\mathbf{V}^{T} \mathbf{c}_{k}^{\dagger} + \mathbf{V}^{S} \alpha_{k})(\mathbf{d}^{T(S)} \mathbf{j}_{d}^{+} \mathbf{j}_{d}^{-})}{\langle (\delta_{d}^{T(S)})_{2} \rangle^{1/2} \langle (\delta_{d}^{T(S)})_{2} \rangle^{1/2}},
$$

which represent the symmetric and antisymmetric combination of coherent transports between the tip and sample via MS, respectively: $(T \rightarrow MS \rightarrow S$: first term) and $(T \leftarrow MS \leftarrow S$: second term) for $\gamma_{TS}^{S}$, and $(T \rightarrow MS \rightarrow S) - (T \leftarrow MS \leftarrow S)$ for $\gamma_{A}^{TS}$. Thus, $\gamma_{A}^{TS}$ vanishes in equilibrium and $\gamma_{A}^{TS} = \gamma_{TS}^{S}$ at steady-state nonequilibrium due to the unidirectional transition of entangled state tunneling. As a result, the first term of $\gamma_{A}^{TS}$ describes figure 3(a).

5. Results

With the reduced Liouville matrix $\mathbf{M}_{r} = \mathbf{c} \mathbf{I} - \mathbf{L}_{a}$ with $\mathbf{z} = -i \omega + \Omega$, we finally arrive at the expression for tunneling conductance,

$$
\frac{df}{dV} = \frac{2e^{2}}{h} \left[ \frac{\Gamma^{S}(\omega)}{\Gamma^{T} + \Gamma^{S}(\omega)} \right] \text{Re} \left( \mathbf{M}_{r}^{-1} \right)_{d_{\delta}d_{\delta}} \bigg|_{\omega = eV}.
$$

Equation (6) gives the tunneling conductance as a function of $\Gamma^{S}(\omega)$ that is proportional to $D(\omega)$. Note that $\Gamma^{S}(\omega)$ appears in both the self-energy matrix $\Sigma$ and the front factor. As it is practically difficult to calculate $\gamma^{S}$ and $\gamma_{TS}^{T}$ for the Hamiltonian given in equation (4), we leave them as free parameters. However, the values of matrix elements is not completely random because each matrix element has its own role. In the previous work [21], we revealed the roles of matrix elements via analytical study for two-reservoir single-impurity Anderson model: matrix elements $\gamma^{T}$ and $\gamma^{S}$ determine the position of the broad side peak and its spectral weight is determined by $\gamma_{A}^{S}$. In contrast, the matrix elements containing Coulomb repulsion $U$ control overall structure of the line shape. In addition, we are able to infer the relative magnitudes of $\gamma_{S}$ by considering the degrees of fluctuation in the metallic tip and superconductor sample. It is reasonable to suppose that fluctuation $\langle (\delta_{d}^{T(S)})_{2} \rangle^{1/2}$ in the tip is bigger than $\langle (\delta_{d}^{T(S)})_{2} \rangle^{1/2}$ in the superconductor, which results in $\gamma^{T} << \gamma^{S}$ because fluctuation appears in the denominator. We apply the same reasoning in choosing the values of $\text{Re}(U_{j}^{T})$ and $\text{Re}(U_{j}^{S})$. However, the steady current condition gives $\text{Re}(U_{j}^{T}) = \text{Re}(U_{j}^{S})$. We set the matrix element values given in table 1 according to this analysis and the condition
Table 1. Values of matrix elements. The values of the matrix elements appearing in \( L_d \) used to obtain figures 4 and 5. We set \( \text{Im}[U_{j-}^T] = 0 \), and all values are in units of \( \Delta_0 \).

| Figure | \( \gamma^T \) | \( \gamma^S \) | \( \gamma^{TS}_{A,L} \) | \( \text{Re}[U_{j-}^T] \) | \( \text{Re}[U_{j-}^S] \) | \( \text{Re}[U_{j-}^{TS}] \) |
|--------|-----------------|--------------|----------------|-----------------|-----------------|-----------------|
| Figure 4 | 0.01 | 0.5 | 0.5 | 0.9 | 6.3 | 4.5 |
| Figure 5 | 0.01 | 0.45 | 0.45 | 0.99 | 3.97 | 2.37 |

Figure 4. (a) Fitting of the experimental tunneling conductance (red line) of single-layer FeSe/STO [2] using flat DOS (green line). The black line is obtained using the values in table 1 and constant DOS of \( \Gamma^T = 0.24\Delta_0 \) and \( \Gamma^S = 1.66\Delta_0 \) with energy unit \( \Delta_0 \).

(b) Fitting of the same experimental tunneling conductance in (a) by varying sample DOS \( \Gamma^j(\omega) \) in the low-energy region of. The sample DOS (magenta + green line) is now composed of a linear-like part (magenta line) and suppressed \( s \)-wave DOS (black dashed line). The grey area indicates the region of flat DOS.

Now, we demonstrate a typical procedure to obtain the DOS function using the STS data for single-layer FeSe/STO [2]. First, we fit the high-bias peak (major peak) of the tunneling conductance using the matrix elements given in table 1 and constant sample DOS for both tip and sample, which gives figure 4(a). All free parameters except \( \Gamma^S(\omega) \) are then fixed with this fitting procedure. Figure 4(a) provides us with the surprising conclusion that the major peak located at 21 meV is not related to the sample DOS. It is just the effect of non-equilibrium entangled state tunneling. Next, we try to fit the low-bias part of the tunneling conductance by varying \( \Gamma^S(\omega) \) in equation (6) to ultimately obtain \( D(\omega) \) (magenta + green line) and a well-fitting tunneling conductance (black line) simultaneously, as shown in figure 4(b). Quantitative agreement up to the high-bias peak is almost exact. The peak of the sample DOS in figure 4(b) is located at 11.9 meV, which coincides with the maximum of the ARPES energy distribution curve [4, 5].

Figure 5. Fitting of the tunneling conductance of Ba$_{1-x}$K$_x$Fe$_2$As$_2$ [6] and extracting sample DOS. The solid black line is our theoretical curve, and the red line is the experimental data. The sample DOS is composed of a linear part (magenta line) at low bias, blue, and green lines. Two \( s \)-wave DOS (black dashed lines: \( \Gamma_1 \) and \( \Gamma_2 \)) are shown with gray dotted tails for ease of viewing. The inset magnifies the crossing area. The grey area indicates the region of flat DOS.

Before presenting the result of our study on extracting the \( s \)-wave DOS functions in Ba$_{1-x}$K$_x$Fe$_2$As$_2$, we analyze the DOS function given in figure 4(b). The line shape of the DOS function will be mostly formed by the band at the M point because the band at the \( \Gamma \) point is suppressed below the Fermi level, as discussed earlier. The magenta line in figure 4(b) represents the contribution by the band at the M point, and the short upright at the top seems to be a weak indirect contribution from the band at the \( \Gamma \) point; we separate it using the black dashed line near the horizontal axis. We conclude that the sample DOS is composed of a linear-type DOS by the band at the M point, and the very much suppressed \( s \)-wave DOS by the band at the \( \Gamma \) point.

Finally, we present the result for Ba$_{1-x}$K$_x$Fe$_2$As$_2$ in figure 5. The value of the experimental tunneling conductance at zero bias is exceptionally non-vanishing [6]. We judge that this non-vanishing at zero bias is not an intrinsic phenomenon, and therefore we study the STS data by considering the minimum at zero bias as the origin of tunneling conductance.

In figure 5, we show the extracted sample DOS (magenta + orange + green line) which contains two \( s \)-wave DOS (black dashed lines indicated by \( \Gamma_1 \) and \( \Gamma_2 \)), although one of them (\( \Gamma_1 \)) is not discernible. The peaks of the \( s \)-wave DOS are located at 5.26 meV and 14.5 meV, which are well
matched with ARPES results [6, 25]. These s-wave DOS correspond to two different Fermi surfaces around the Γ point: the outer Fermi surface (Γ2) produces a pronounced s-wave peak at lower energy, while the inner Fermi surface (Γ1) generates a lower s-wave peak at higher energy. An additional Fermi level. In contrast, the two incoherent Coulomb peaks can be seen in various mesoscopic quantum impurity systems [26, 27]. However, the zero-bias peak is suppressed in the case of strong asymmetry in coupling strength, i.e. γ2 ≪ γ5, or when sample DOS has a gap or vanishes at the Fermi level. In contrast, the two incoherent Coulomb peaks are present far outside the concerned energy range. Thus, the two additional low-energy coherent peaks remain alone in the tunneling conductance of correlated superconductors. The low-energy coherent peak appears as a major peak in STS data and is misunderstood as a superconducting peak [24]. We stress here that the major peak shown in the STS data is solely an effect of nonequilibrium, being a unique feature of entangled state tunneling under bias. The sample DOS of a correlated superconductor is not usually prominent in the STS line shape; therefore, a theoretical formula relating tunneling conductance and sample DOS is necessary to extract the sample DOS from tunneling data. Equation (6) plays this role. To extract a reliable sample DOS using equation (6), high-quality STS data are required.

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6. Discussion

We have revealed ordinary s-wave DOS of Fe-based superconductor Ba1-xKxFe2As2 hidden in the tunneling conductance. We adopted the Liouville approach in which a complete set of basis vectors (operators) can be determined. The infinite-dimensional Liouville matrix is reduced to a 5 × 5 matrix yielding five general peaks in local DOS ρd(ω): one coherent peak at the Fermi level, two additional low-energy coherent peaks, and two incoherent Coulomb peaks. The three coherent peaks can be seen in various mesoscopic quantum impurity systems [26, 27]. However, the zero-bias peak is suppressed in the case of strong asymmetry in coupling strength, i.e. γ2 ≪ γ5, or when sample DOS has a gap or vanishes at the Fermi level. In contrast, the two incoherent Coulomb peaks are present far outside the concerned energy range. Thus, the two additional low-energy coherent peaks remain alone in the tunneling conductance of correlated superconductors. The low-energy coherent peak appears as a major peak in STS data and is misunderstood as a superconducting peak [24]. We stress here that the major peak shown in the STS data is solely an effect of nonequilibrium, being a unique feature of entangled state tunneling under bias. The sample DOS of a correlated superconductor is not usually prominent in the STS line shape; therefore, a theoretical formula relating tunneling conductance and sample DOS is necessary to extract the sample.