

Two-step method for tracing the density of states from scanning tunneling spectra

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We present a two-step deconvolution algorithm for recovering the density of states (DOS) of the sample from scanning tunneling spectroscopy measurements without requiring prior knowledge of the tip state. The method first uses the DOS and the dI/dV spectrum of a known feature to characterize the product of the DOS of a tip and the tunneling probability. With this product and the dI/dV spectrum measured on the sample with the same tip, the DOS of the sample can be further derived. Applied to both simulated and experimental data on engineered quantum corrals, as well as the adatoms placed inside them, the algorithm exhibits robust reproducibility under various tip conditions and uncovers subtle modulations of adatom resonance states related to quantum confinement and inversion effects. By extracting a high-fidelity DOS, the method offers a powerful approach for investigating artificial nanostructures and the related quantum phenomena.

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I. INTRODUCTION

The density of states (DOS), which quantifies the number of available electronic states per unit of energy, is a crucial bridge linking microscopic quantum states to the macroscopic properties of materials. It plays an essential role in understanding emerging phenomena [1–8], engineering material properties [9–13], designing advanced devices [14–16], and optimizing their performance. In theory, the DOS can be calculated with various band structure calculation tools. In experiment, it can be probed via several techniques, such as photoemission spectroscopy and scanning tunneling spectroscopy (STS), with the latter enabling the investigation of the local DOS (LDOS) down to atomic scale. It sounds like a dream combination as the joint interplay between experiment and theory is expected to advance the field significantly. STS, however, typically measures only the differential conductance spectrum (dI/dV) rather than the LDOS directly [17–20]. How to trace the LDOS from the dI/dV spectrum is thus an outstanding problem in the community [21–30].

The main difficulty is that the dI/dV spectrum not only contains information about the LDOS of the sample but is also influenced by various factors, such as the work functions of both the tip and the sample, the electronic structure

of the tip, the tip-sample distance, and the temperature. In addition, the LDOS is superimposed on an exponentially dependent background caused by the tunneling, and the tip information is practically unknown, making the extrapolation of the LDOS even more difficult. Moreover, the tips differ for different batches of experiments, and they exhibit different electronic states, complicating the data analysis. Several different approaches have been applied to extrapolate the LDOS from the measured spectra. They can be roughly categorized into three types. The first one closely resembles a fitting procedure, in which the DOS of the tip ρ_T and the DOS of the sample ρ_S are modeled with the use of specific forms. These forms are typically constants or analytically defined expressions [21,23,28,30], with only a few parameters awaiting extraction through curve fitting. This approach is viable only when the format of both ρ_T and ρ_S is clearly known in advance, strongly limiting its application. The second category aligns more closely with the experimental intuition. Instead of explicitly modeling ρ_T , these methods leverage the well-characterized surface states of two-dimensional electron gases (2DEGs) to recover ρ_S in systems involving Kondo resonance [27] or quantum corral studies [31]. Its generalizability, however, is limited in cases involving nonconstant ρ_T . The third approach has been implemented by solving the model self-consistently [25,26,29], wherein STS data acquired at multiple different tip-sample distances are used to formulate and iteratively solve a set of equations, allowing the

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recovery of the LDOS of the sample from the STS spectra. The inclusion of sufficient STS datasets and corresponding height information ensures robust parameter resolution, although this inevitably increases experimental complexity due to the need for customized STS measurements. The extension based on this method uses constant-current STS to capture the height variations. The results, however, often do not align well with those obtained from constant-height STS, suggesting that the tunneling probability function may be more complex than commonly assumed [22,24]. In short, the methods mentioned above either assume a specific form of the tip LDOS and the sample LDOS or require additional complex measurements. This necessitated an approach that better aligns with experimental practice to increase the reliability of data interpretation and ensure consistency across different measurements.

In this work, we present a two-step deconvolution algorithm that minimizes the assumptions made and the demand for additional data, while maintaining the tracing accuracy of the LDOS. In our approach, we use two primary strategies to simplify the deconvolution process. First, instead of solving both ρ_T and the tunneling transmission probability T , we calculate only their product, which we name the “tip-related tunneling function” κ_T . In this way, we reduce the parameters that need to be calculated. Second, we use a reference LDOS of a known feature ρ_R and its measured dI/dV spectrum σ_R to characterize κ_T of an unknown tip on top of the feature. The same tip is then used to probe the target sample in almost the same tunneling conditions, and the dI/dV spectrum obtained is further used to trace the sample LDOS with the aid of the previously determined κ_T . In this way, our approach can perform deconvolution of the LDOS from the dI/dV spectra even in the presence of complex tip states. We demonstrate our method with both simulated and experimental datasets. The one-to-one correspondence obtained between the deconvolved LDOS and the presets, or the LDOS calculated with Green’s function theory, unambiguously evidences the robustness and reliability of the method. Our approach thus provides a powerful tool for studying artificial nanostructures and related quantum phenomena.

II. BASICS OF THE DECONVOLUTION ALGORITHM

A. Small-bias approximation

We consider a typical STM configuration in which the tip is grounded and a bias voltage is applied to the sample (the inverse setup is mathematically equivalent), and assume negligible perturbation from the tip to the sample. Under conditions where the thermal energy $k_B T$ and the modulation voltage V_{mod} used for spectroscopy measurements satisfy $k_B T \ll V_{\text{mod}}$, the measured dI/dV under the

constant-height condition can be expressed as

$$dI/dV(V) \propto \frac{d}{dV} \int_0^{eV} \rho_S(\varepsilon) \rho_T(\varepsilon - eV) T(\varepsilon, V, d) d\varepsilon, \quad (1)$$

where the tunneling transmission probability $T(\varepsilon, V, d)$ depends on the wave functions of the tip and the sample, as well as the tip-sample separation d . Among the various approaches to LDOS deconvolution, a widely adopted framework is an approximate theory that extends the Tersoff-Hamann model by incorporating a one-dimensional Wentzel-Kramers-Brillouin (WKB) formalism with a trapezoidal barrier [18,19]. Recovering the sample’s density of states $\rho_S(\varepsilon)$ from the measured dI/dV spectrum thus amounts to solving an ill-posed Volterra-type integral equation. The primary difficulty in this process lies in the fact that both ρ_T and the tunneling transmission probability $T(\varepsilon, V, d)$ are generally unknown. If one wants to treat the entire kernel $\rho_T(\varepsilon - eV) T(\varepsilon, V, d)$ as a matrix in a direct optimization routine, the problem becomes computationally unstable, and convergence is often unachievable. Hence, a tunneling transmission probability can be expressed as:

$$T(\varepsilon, V, d) \propto \exp \left[-2d(2m_e)^{1/2} \hbar^{-1} \sqrt{\Phi_{\text{av}} - \varepsilon + eV/2} \right],$$

where Φ_{av} is the average work function of the probed surface and the tip, and m_e is the mass of the electron. This is derived from the WKB approximation under the assumptions of a tip with s -wave electronic state and a trapezoidal potential barrier. This formulation provides a convenient starting point. Although the constraint imposed by the tunneling transmission function derived from the WKB model may seem to improve the feasibility of convergence, the solution remains nonunique without additional information regarding the tip-sample distance and the work functions of both the tip and the sample. In real experiments, the tunneling process can involve factors that are far more complex. And it is not straightforward to capture these contributions with the use of a simple approximation.

Here we also use the tunneling current formalism originally proposed by Tersoff and Hamann [18]. Differently, we do not use the widely adopted s -wave approximation. As the most essential physical quantity in this model is the momentum $\kappa_0(\varepsilon, V) = (2m_e)^{1/2} \hbar^{-1} \sqrt{\Phi_{\text{av}} - \varepsilon + eV/2}$, the tunneling function can be generally expressed as $T(\varepsilon, V, d) \propto \sum_l c_l(\varepsilon - eV) \exp[-2\kappa_0(\varepsilon, V)d]$ when the contributions from the tip geometry and the different orbitals of the apex atom are included [32]. In it, c_l encodes the geometric and orbital-dependent factors associated with the tip electronic structure. We further define a dimensionless variable $x = eV/(2[\Phi_{\text{av}} - (\varepsilon - eV)])$, allowing us to expand the tunneling transmission function as a series in x :

$$\begin{aligned}
T(\varepsilon, V, d) &\propto \sum_l c_l(\varepsilon - eV) \exp \left[-2d \frac{\sqrt{2m_e}}{\hbar} \sqrt{\Phi_{av} - (\varepsilon - eV)} \sqrt{1-x} \right] \\
&\approx \sum_l c_l(\varepsilon - eV) \exp \left[-2d \frac{\sqrt{2m_e}}{\hbar} \sqrt{\Phi_{av} - (\varepsilon - eV)} \left(1 - \frac{x}{2} + \dots \right) \right].
\end{aligned} \tag{2}$$

Since the work function of noble metals typically exceeds 4 eV and x varies slowly around the Fermi level, a first-order expansion of Eq. (2) is typically sufficient in small-bias regimes, allowing the transmission probability T to be primarily treated as

$$T \propto \sum_l c_l(\varepsilon - eV) \exp \left[-2d \left(1 - \frac{x}{2} \right) \frac{\sqrt{2m_e}}{\hbar} \sqrt{\Phi_{av} - (\varepsilon - eV)} \right],$$

which is a function of $\varepsilon - eV$. In comparison with the result derived with use of the WKB approximation, $T(\varepsilon, V, d)$ obtained with our approach is effectively shifted by $eV/2$. When V is much smaller than Φ_{av} , the impact of this shift is rather limited. This, however, offers a mathematical advantage in the analysis, as will be further discussed below.

In larger-bias ranges, higher-order effects become non-negligible, leading to slight deviations in the deconvolved results. Here we introduce an effective tip-sample distance $\tilde{d}$, which serves as a compensatory parameter capturing the effect of this approximation. In practice, variations in tip geometry and the orbital character of the tip wave function can lead to different tunneling transmission functions, which are not fully captured by the WKB model and cannot be quantitatively described within its framework. However, the approximation used here remains applicable to other situations where the work function is significantly larger than the measurement bias range. Under this condition, we derive a tunneling transmission function $T(\varepsilon - eV, \tilde{d})$ that can be expressed as a function of $\varepsilon - eV$. At the same time, by normalizing the measured dI/dV curve with its value at zero bias, we can reduce the influence of both the effective tip-sample distance $\tilde{d}$ and the work function Φ_{av} (see note 1 in Supplemental Material [33]). In addition, this kind of normalization makes the normalized values near zero bias close to 1 and brings the normalized spectrum into an algorithm-friendly range and prevents numerical overflow during optimization. This normalization is valid only for systems with a considerable zero-bias value in the dI/dV spectrum. In systems where the zero-bias value is small, such as superconducting or semiconducting samples, other normalization choices are possible, but they typically require manual rescaling of the final deconvolved spectra.

As shown in Eq. (1), although both ρ_T and $T(\varepsilon - eV, \tilde{d})$ are unknown, only their product is the essential factor that determines the dI/dV spectrum besides the LDOS of the sample. Thus, we define an effective tip-related tunneling function $\kappa_T(\varepsilon)$ as their product, i.e., $\kappa_T(\varepsilon) = \rho_T(\varepsilon)T(\varepsilon, \tilde{d})$,

to simplify the deconvolution process. In this way, we transform the original integral equation [Eq. (1)] into a more tractable form:

$$\sigma_w(V) \propto \frac{\partial}{\partial V} \int_0^{eV} \rho_w(\varepsilon) \kappa_T(\varepsilon - eV) d\varepsilon \quad (w = R, S). \tag{3}$$

This formula serves two important functions in our two-step deconvolution process. In the first step, we set $w = R$. In such a case, σ_w and ρ_w represent the measured dI/dV spectrum and the LDOS of a reference feature, respectively. Equation (3) serves to derive the effective tip-related tunneling function $\kappa_T(\varepsilon)$. In the second step, we set $w = S$. In such a case, σ_w and ρ_w represent the measured dI/dV spectrum and the LDOS of the target sample, respectively. With $\kappa_T(\varepsilon)$ obtained in the first step, Eq. (3) further serves to calculate the LDOS of the target sample ρ_S .

It is worth mentioning that this is *not* equivalent to assuming a constant tunneling matrix element. Instead, it encodes the physics of tunneling within a physically informed kernel function. Furthermore, since the actual tip-sample coupling is strongly influenced by local variations in both the sample's electronic structure and the tip geometry, this formulation does not strictly require the transmission to follow the WKB approximation. Still, it remains valid in scenarios where the average work function Φ_{av} greatly exceeds the experimental bias range and the same atomic species is probed. Thus, by introducing physically motivated constraints from Eq. (3), our approach successfully bypasses the need for detailed knowledge of the LDOS of the actual tip or the exact tip-sample coupling, thus greatly reducing the complexity of solving the otherwise ill-posed Volterra integral equation. While this approach is appropriate for the present dataset, it is not intended for systems in which the intrinsic spectral width is comparable to or smaller than $k_B T$. Examples include STM measurements of superconducting gaps or submilli-electronvolt inelastic features [34,35], where temperature-dependent broadening must be retained in the tunneling formalism and the lock-in influence cannot be simplified.

B. Two-step optimization scheme

Our algorithm is designed to accommodate the deconvolution of the sample LDOS even in cases where the reference LDOS ρ_R displays complexities. Leveraging recent advances in nonlinear optimization, particularly the efficiency of algorithms such as the L-BFGS-B algorithm [36–38], we construct a fast and robust two-step optimization scheme to iteratively determine the effective tip-related tunneling function κ_T that best satisfies the imposed physical constraints (see Fig. 1). Under the small-bias approximation discussed above, the discretized form of the measured dI/dV spectra, which are sampled uniformly over the interval $[-U, U]$ at $2n_0 + 1$ points (we consider the case of an odd number of points for simplicity), can be expressed as a system of linear equations:

$$\begin{cases} \sigma_R = \mathbf{A}[\rho_R]\kappa_T, \\ \sigma_S = \mathbf{B}[\kappa_T]\rho_S. \end{cases} \quad (4)$$

Here the tip-related tunneling function κ_T and the target sample LDOS ρ_S are unknown and await determination. The matrix $\mathbf{A}$ is constructed with the use of a known reference feature LDOS ρ_R (e.g., the LDOS of an idealized

surface state of 2DEGs or an isolated atom on a wide terrace), while $\mathbf{B}$ is constructed from optimal κ_T given by the first line of Eq. (4). σ_R and σ_S are the measured dI/dV spectra of a known reference feature and the unknown target sample, respectively. This inverse problem is inherently ill-posed: the matrix $\mathbf{A}$ is not guaranteed to be invertible, and a pseudoinverse often yields spurious oscillations as the solution is highly sensitive to noise. Similar difficulties are encountered in image deconvolution problems, where techniques such as the Kalman filter [39] and the Wiener filter [40–44] are commonly used. In our approach, we use Tikhonov-Phillips regularization (TPR) [45,46] to stabilize the inversion and guide the search for physically meaningful κ_T and ρ_S . During practical measurements, each sample LDOS acquisition is accompanied by at least one reference STS measurement before and after, ensuring that the tip-related tunneling function κ_T remains stable throughout the process. Indeed, we find that even after acquiring several dozen STS spectra, the final reference spectrum remains virtually indistinguishable from the initial one, confirming the robustness and reproducibility of the tip condition during the experiment.

As shown in Fig. 1, the first step of our algorithm takes the reference LDOS and its corresponding measured dI/dV

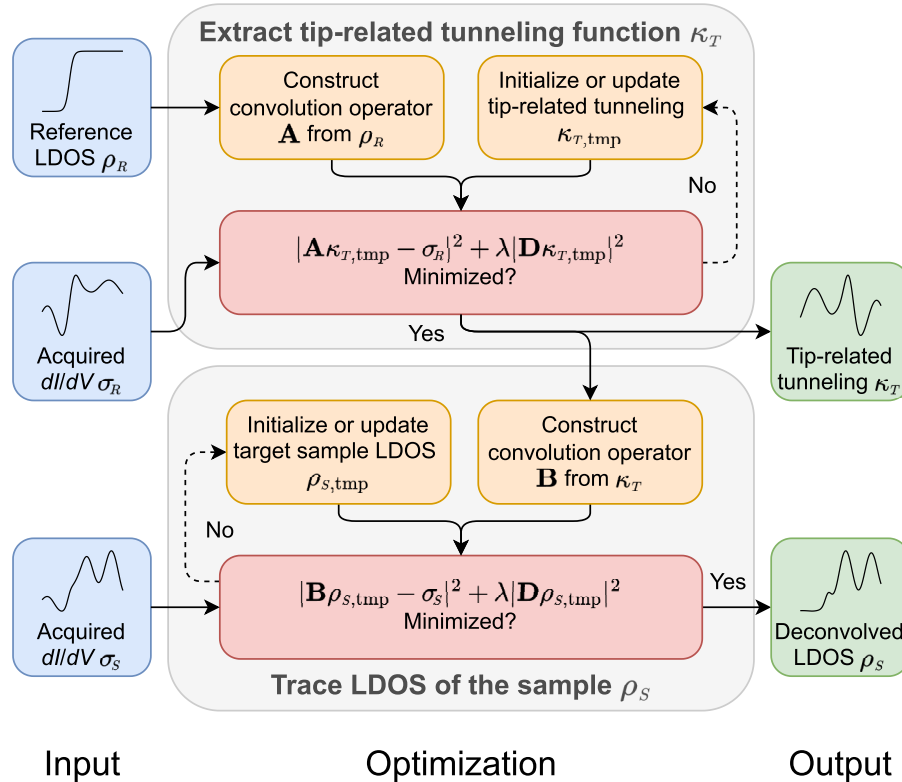


FIG. 1. The two-step algorithm for tracing the LDOS from the scanning tunneling spectra. To deconvolve the LDOS of a target sample ρ_S , the dI/dV spectra of the target sample σ_S and a known reference feature σ_R are measured with the same STM tip. The reference feature has a known referenced LDOS ρ_R . In the first step, the combination of ρ_R and σ_R is used to calculate the effective tip-related tunneling function κ_T , based on an optimization algorithm. In the second step, the obtained κ_T together with σ_S is further used to deconvolve ρ_S on the basis of a similar optimization algorithm. Subscript “tmp” indicates temporary variables during iteration.

spectrum as the input to derive κ_T . The reference LDOS ρ_R is used to construct the matrix $\mathbf{A}$, and an initial trial for κ_T is generated. By multiplication of $\mathbf{A}$ and κ_T , the residual is computed with respect to the experimentally measured reference spectrum σ_R . To enforce physical smoothness, we introduce a TPR term involving a first-order difference matrix $\mathbf{D}$, with a regularization parameter λ controlling the strength of the regularization:

$$\mathcal{L} = |\sigma_R - \mathbf{A}\kappa_T|^2 + \lambda|\mathbf{D}\kappa_T|^2. \quad (5)$$

Although λ is an empirical parameter, we find that values on the order of 10^{-4} typically suffice for high-quality data, balancing fidelity to the measurement with smoothness of the solution. The optimal κ_T is obtained by minimizing the total loss function $\mathcal{L}$ using an efficient iterative optimization algorithm, such as the L-BFGS-B algorithm. In

the second step of our algorithm, a new matrix $\mathbf{B}$ is constructed with the use of the previously determined κ_T , and the optimization is now performed over ρ_S . The deconvolved density of states is defined as the solution that satisfies a predefined convergence criterion, typically when the residual falls below a threshold value.

III. RESULTS AND DISCUSSION

A. Test on a simulated dataset

We first test our method with a simulated dataset where both the LDOS of a reference feature and a sample, $\rho_R(\text{truth})$ and $\rho_S(\text{truth})$, are preset and will be used to cross-check the output. Figure 2 illustrates the deconvolution process and the results. Although $\rho_R(\text{truth})$ [dashed black line in Fig. 2(a)] is a steplike function, mimicking the LDOS of a Ag (111) surface, the dI/dV spectrum, $\sigma_R(\text{sim.})$

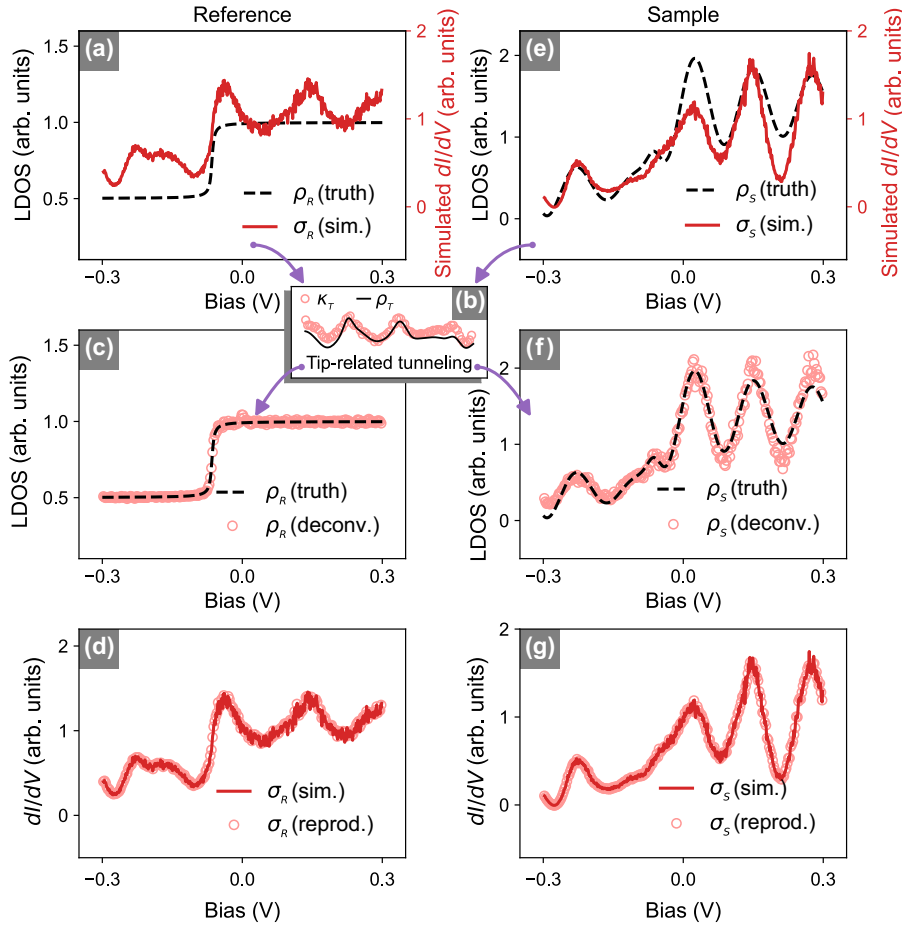


FIG. 2. Deconvolution process with the simulated data. (a) Simulated dI/dV data (red curve, generated with a complex tip LDOS ρ_T at $d = 1.6$ nm and a signal-noise-ratio of 25) and the reference LDOS $\rho_R(\text{truth})$ (dashed black line). (b) Derived tip-related tunneling function κ_T (open red circles) and the DOS of the tip ρ_T (black line). (c) Comparison of the deconvolved reference LDOS $\rho_R(\text{deconv.})$ (pink circles) and the reference LDOS $\rho_R(\text{truth})$ (dashed black line). (d) Comparison of the reproduced and simulated dI/dV spectra, $\rho_R(\text{deconv.})$ (open red circles) and $\sigma_R(\text{sim.})$. The reproduced spectrum $\sigma_R(\text{reprod.})$ is calculated from the deconvolved result. (e)–(g) The same procedure is applied to deconvolve the sample LDOS containing unknown spectral features with the derived tip-related tunneling function κ_T shown in (b).

[solid red line in Fig. 2(a)], shows a very different and complex feature with multiple peaks as a poorly treated tip is assumed. Although this type of $\sigma_R(\text{sim.})$ is far from ideal, it is often found in real experiments. Note that the dI/dV spectrum is generated under a tip-sample separation d of 1.6 nm and an average work function of 4 eV. In addition, random noise is added to simulate an uncertainty of approximately 4%. By applying the deconvolution procedure to the input shown in Fig. 2(a), we extract the optimal κ_T [pink circles in Fig. 2(b)], which incorporates both the original tip DOS ρ_T and the contributions from the tunneling matrix elements. For comparison, we also plot the preset ρ_T [black line in Fig. 2(b)] that was used to calculate $\sigma_R(\text{sim.})$ shown in Fig. 2(a). It shows an apparent similarity with κ_T near the Fermi level but deviates at larger-bias regions due to variations in the tunneling barrier. Figure 2(c) provides a comparison of the deconvolved reference LDOS and the reference LDOS, $\rho_R(\text{deconv.})$ (open pink circles) and $\rho_R(\text{truth})$ (dashed black line). They exhibit almost identical curves, indicating the successful derivation of κ_T . To further confirm this, we also calculated the dI/dV spectrum $\sigma_R(\text{reprod.})$ using $\rho_R(\text{deconv.})$ and κ_T , and compared it with the simulated one $\sigma_R(\text{sim.})$. The results obtained [see Fig. 2(d)] show excellent agreement, once again confirming the successful generation of κ_T .

Next we further test the method on the sample of interest. Figure 2(e) shows the preset sample LDOS $\rho_S(\text{truth})$ (dashed black line) and the simulated dI/dV spectrum $\sigma_S(\text{sim.})$ (solid red line). They are apparently different. With κ_T obtained from the first step and $\sigma_S(\text{sim.})$, we deconvolve the sample LDOS $\rho_S(\text{deconv.})$, which exhibits close similarity with $\rho_S(\text{truth})$ also plotted in Fig. 2(f). As shown in Fig. 2(g), the reproduced dI/dV spectrum $\sigma_S(\text{reprod.})$ also matches well with $\sigma_S(\text{sim.})$, confirming the successful deconvolution. To cross-check the robustness of our two-step method, we conducted several additional tests. With several different ρ_T values as inputs, we find that almost the same $\rho_S(\text{deconv.})$ can be generated. And with several different $\rho_S(\text{truth})$, the deconvolved sample LDOS $\rho_S(\text{deconv.})$ exhibits remarkable similarity with the corresponding input $\rho_S(\text{truth})$. These results demonstrate the generality and reliability of our deconvolution method.

B. Quantum corrals

The numerical validation based on the simulated measurements demonstrates the robustness of our deconvolution algorithm under complex conditions, and its practical utility is further confirmed through application to real experimental data. In our experiments (Fig. 3), Fe adatoms were deposited onto a clean Ag(111) surface at a temperature of approximately 6 K. Within the same atomically flat region, three circular quantum corrals with radii of 3.2, 5.1, and 9.2 nm were fabricated with Fe adatoms

by atom manipulation at well-separated positions in a single session. Under the same tip condition, dI/dV spectra were sequentially acquired on the bare Ag(111) surface and at the centers of the three corrals—each confining the surface state to different features. The STS measurements were taken in ultrahigh vacuum at a temperature of approximately 4.7 K. Throughout the measurements, the differential conductance spectra were acquired with a standard lock-in detection method with a modulation voltage $V_{\text{mod}} = 4$ mV applied to the sample at a frequency of 6.778 kHz. The choice of lock-in frequency depends on the signal-to-noise ratio and the bandwidth of the current amplifier. We also performed measurements at both 666 Hz and 6.778 kHz for comparison. The spectra obtained are essentially the same within the experimental error margin (see note 2 in Supplemental Material [33]). For each position, 25 spectra were repeatedly collected and averaged. Following each set of measurements, the tip was modified arbitrarily, and the surface state STS spectrum was remeasured to confirm an apparent change in the tip condition, thereby initiating a new acquisition round if a distinct tip DOS was found. In total, three distinct tip conditions were sampled, as shown with different colors in Figs. 3(a), 3(c), 3(e), and 3(g). Figures 3(b), 3(d), 3(f), and 3(h) present the corresponding deconvolved datasets obtained with our algorithm, as detailed above. In the deconvolution process, the theoretical Ag(111) surface state LDOS with a bulk state background served as the reference. The reference LDOS model is adopted as an arctangent-type function and incorporates bulk contributions [47], taking the form $3/4 + (2\pi)^{-1} \arctan[(eV - E_0)/2\Gamma_0]$, where $\Gamma_0 = 7$ meV and $E_0 = -67$ meV, corresponding to the onset energy of the Ag(111) surface state.

Following the deconvolution process, the recovered sample LDOS under all three tip conditions exhibits remarkable consistency, indicating that the tip-induced variation has been effectively removed. This confirms the high reproducibility of the spectra after correction for the tip effects. To compare the deconvolved spectra with theory, we perform calculations based on the Green's function multiple-scattering formalism, evaluating the LDOS at the corral centers via $\rho_S(\varepsilon) = -\pi^{-1} \text{Im}[G(\varepsilon + i\text{Im}\Gamma)]$, where the imaginary part of the self-energy $\text{Im}\Gamma = \beta + \gamma(E - E_F)^2$ accounts for lifetime broadening due to surface state scattering [48–50]. Here, $\beta = 5$ meV and γ is a parameter depending on the corral size and adatom density of the wall [31]. γ is 0.299, 0.382 and 0.718 eV⁻¹ for the corrals with radii of 3.2, 5.1, and 9.2 nm, respectively. In all calculations, the scattering potential is fixed as $V_{\text{scatter}} = (-0.218 - 0.259i)\rho_0^{-1}$, where ρ_0 represents the constant LDOS of the 2DEG. Special care must be taken to handle potential artifacts when steplike reference LDOS profiles are used in deconvolution. While our algorithm does not explicitly perform fast Fourier transforms, which would introduce possible zero-division issues, implicit

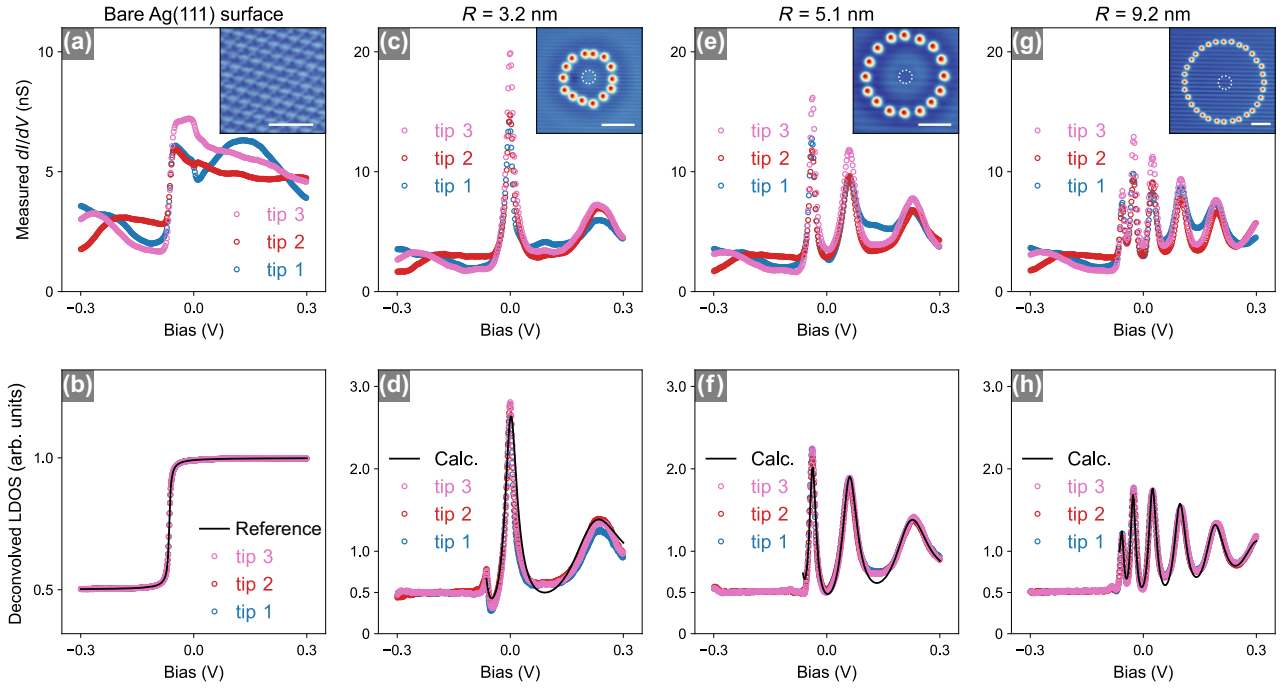


FIG. 3. Deconvolution of the quantum well states measured in different-sized quantum corrals formed by Fe adatoms on the Ag(111) surface. (a),(c),(e),(g) STS spectra taken with three different tips (blue, red, and pink) on a wide Ag(111) terrace and at the center of circular corrals with radii R of 3.2, 5.1, and 9.2 nm, respectively. (b),(d),(f),(h) Corresponding deconvolved results for each case, plotted in corresponding colors. In (b), the reference LDOS of the Ag(111) surface state (solid black line) is modeled by an arctangent-type function with a broadening parameter $\Gamma_0 = 7$ meV, combined with a bulk contribution. In (d),(f),(h), the solid black lines represent the results calculated with the use of a multiscattering Green's function approach.

Fourier components are unavoidable during optimization. Therefore, sharp discontinuities such as step edges or truncation at finite signal length may give rise to Gibbs phenomena, manifesting themselves as nonphysical oscillations in the recovered LDOS. These artifacts can be mitigated by stronger regularization (i.e., increasing λ) or suppressed with the use of neural network-based postprocessing techniques [51].

C. Inversion effect in quantum corral

Up to this point, we have validated our deconvolution algorithm using the dI/dV spectra obtained at the centers of quantum corrals, with the surface state LDOS measured on a wide terrace serving as a reference. In the context of engineered nanostructures, the dI/dV spectra acquired atop the individual adatoms are also of great importance. To explore this, we placed an additional Fe atom at the center of a quantum corral with $R = 5.1$ nm and repeated the measurement procedure by acquiring dI/dV spectra under two distinct tip conditions [Fig. 4(c)]. As discussed in Ref. [52], the modulation in Fig. 4(d) originates from an inversion effect. In contrast to previous cases, the reference dI/dV spectrum here was taken from an isolated Fe adatom on the bare Ag(111) surface [Fig. 4(a)]. Such a choice ensures that the tunneling occurs in between the

tip and the atom of the same element. In this condition, the tunneling matrix elements may remain almost consistent between reference and target spectra. This is of critical importance, since different tunneling geometries can otherwise compromise the reliability of the deconvolution process. The reference LDOS is obtained by our fitting high-quality dI/dV data from an isolated Fe adatom on the bare Ag(111) surface using the analytical model proposed in Ref. [47]. After application of the deconvolution algorithm, the deconvolved LDOS of the Fe atom placed at the center of the quantum corral becomes almost identical to each other, as shown in Fig. 4(d), despite the dI/dV spectra from the two measurements showing an apparent difference since two different tips were used. We calculated the LDOS using the dressed Green's function [50,53] by combining the numerically computed Green's function of the $R = 5.1$ nm empty corral in Fig. 3(f) with a theoretical model of the resonance from Ref. [47]. The detailed calculation is presented in note 4 in Supplemental Material [33]. The result shows that the deconvolved spectra, obtained with the theoretical single-atom resonance model as the reference LDOS, match well with the model prediction within the same theoretical framework. This self-consistency demonstrates that our deconvolution algorithm enables the deconvolved signals to be consistently interpreted within a unified theoretical

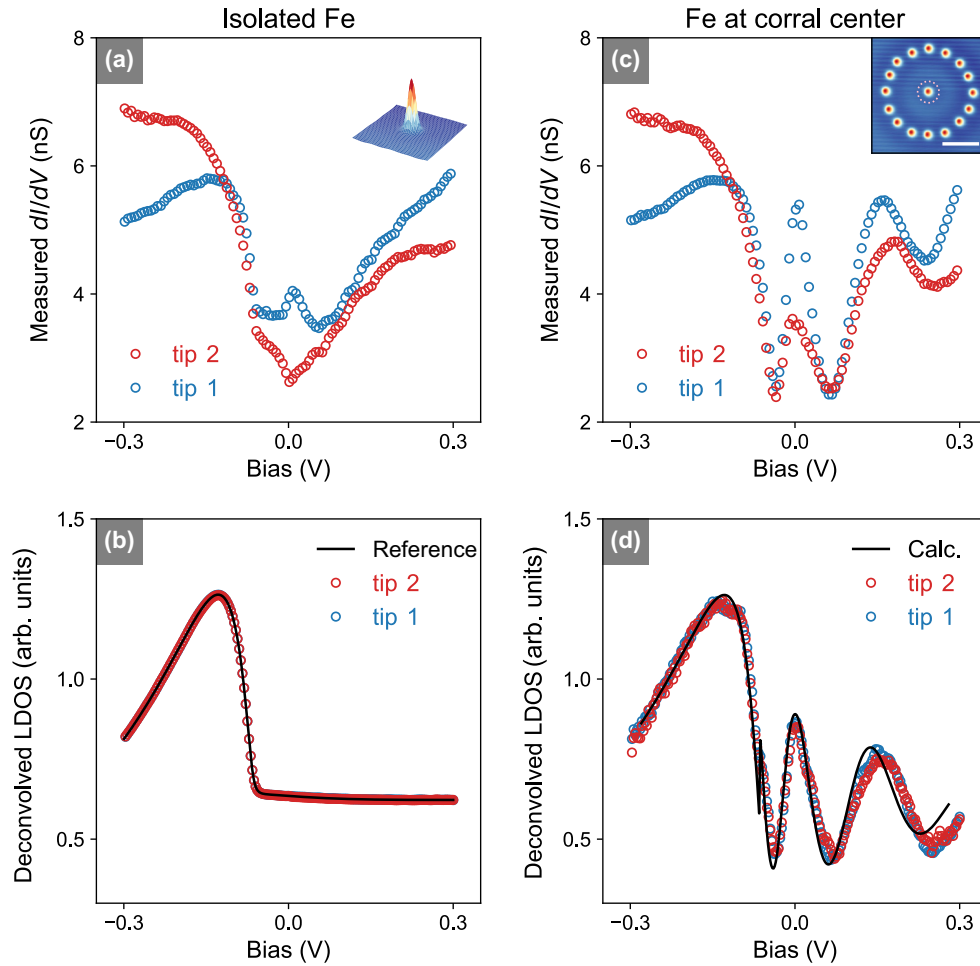


FIG. 4. Deconvolution of LDOS from the STS spectra measured at Fe adatoms positioned at the centers of quantum corrals on the Ag(111) surface. (a),(c) STS spectra taken on an isolated Fe adatom and on top of an Fe adatom placed at the center of a circular corral with $R = 5.1$ nm, using two different tips (blue and red). (b),(d) Corresponding deconvolved results, plotted in matching colors. In (b), the reference DOS of the isolated Fe adatom (solid black line) is modeled with the use of an established analytical form from Ref. [47]. In (d), the solid black lines represent theoretical results calculated with a Green's function approach [50,53].

framework, thereby significantly enhancing the reusability of the experimental data and increasing the overall self-consistency between theory and experiment.

Above, we showed the successful deconvolution using a normal metallic tip, such as a W or Pt-Ir tip. In superconductor-related research, superconducting tips are commonly used to increase the energy resolution. Using simulations, similarly to what we did in Fig. 2, we show our algorithm can also be used for the cases of using superconducting tips to probe the superconducting gaps and the in-gap Yu-Shiba-Rusinov states of magnetic single adatoms on a superconducting substrate (see note 5 in Supplemental Material [33]). Although its feasibility still needs to be experimentally verified, it shows strong potential in the study of superconducting materials.

In our deconvolution algorithm, the choice of the reference LDOS plays a critical role. While the reference LDOS in certain systems, such as a 2DEG, is well known,

it may not be as straightforward in more complex scenarios. In practice, however, a single high-quality and trustworthy measurement can also serve as a suitable reference [33]. Since it is impossible to obtain the LDOS experimentally without involving the tip, conventional tip conditioning procedures already rely on characteristic dI/dV spectra—such as those from 2DEG-like systems—to assess the tip state. Owing to the linearity of the convolution process in dI/dV spectra, the two-step deconvolution algorithm enables the use of a prior measurement from the same sample as the reference “LDOS.” In doing so, the tip state from that reference is effectively “transferred” to the current measurement, ensuring consistency across different experimental sessions. In other words, the two-step algorithm allows data acquired at various times to be aligned with a chosen reference measurement, thereby facilitating the reuse of cross-experimental data, although the real LDOS still needs to be further determined.

IV. SUMMARY

We have developed and validated a two-step deconvolution algorithm to recover the LDOS from dI/dV spectra measured with STM, accounting for complex tip states and tunneling matrix elements. The method is based on a physically motivated approximation of the tunneling transmission, transforming the inversion of the ill-posed Volterra integral equation into a tractable regularized optimization problem. Using simulated and real experimental data collected from quantum corrals of various sizes, with and without adatoms placed within them, we demonstrate that the algorithm can robustly eliminate tip-induced artifacts and produce highly reproducible results across different tip conditions. Notably, we observe weak but discernible modulations of Fe adatom resonances due to confinement-induced inversion effects. These findings establish the algorithm as a powerful and practical tool for high-fidelity LDOS analysis in STS experiments, especially in the context of artificial nanostructure engineering. We expect the framework may be further extended to spin- and orbital-resolved STM measurements, offering a promising avenue for deconvolving complex tunneling signals in emerging spintronic and quantum materials. We also note that line-shape distortions associated with the lock-in detection process or with the electromagnetic environment of the STM, as reported in Refs. [34,35], lie outside the scope of our present formulation. Such effects require a full temperature-dependent treatment in combination with a device-specific model of environmental coupling.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

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