Quasiparticle density of states by inversion with maximum entropy method

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We propose to extract the quasiparticle density of states (DOS) of the superconductor directly from the experimentally measured superconductor-insulator-superconductor junction tunneling data by applying the maximum entropy method to the nonlinear systems. It merits the advantage of model independence with minimum *a priori* assumptions. Various components of the proposed method have been carefully investigated, including the meaning of the targeting function, the mock function, as well as the role and the designation of the input parameters. The validity of the developed scheme is shown by two kinds of tests for systems with known DOS. As a preliminary application to a $Bi_2Sr_2CaCu_2O_{8+\delta}$ sample with its critical temperature $T_c = 89$ K, we extract the DOS from the measured intrinsic Josephson junction current data at temperatures of $T = 4.2$ K, 45 K, 55 K, 95 K, and 130 K. The energy gap decreases with increasing temperature below T_c, while above T_c, a kind of energy gap survives, which provides an angle to investigate the pseudogap phenomenon in high-T_c superconductors. The developed method itself might be a useful tool for future applications in various fields.

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I. INTRODUCTION

It has been more than two and a half decades since the seminal discovery of high-temperature superconductivity in cuprates [1]. In spite of the enormous progress made in materials synthesis, crystal growth, experimental studies of physical properties, and theoretical interpretation, there is still no consensus regarding the superconductivity mechanisms, in association with the so-called "pseudogap" phenomena [2], in these cuprate compounds.

The study of the quasiparticle density of states (DOS) plays a central role in condensed matter physics, especially in strongly correlated many-body systems including high-temperature superconductors. In this paper, we propose to extract the electronic DOS from the directly measured $I(V)$ curve data of a superconductor-insulator-superconductor (SIS) tunneling junction [3] with the application of the maximum entropy method [4–10]. The advantage of such an approach is that it is model-independent with minimum *a priori* assumptions.

It is expected and desirable to apply such an inversion method to the existing experimental data of the SIS tunneling junction, and to interpret the underlying physics of the extracted DOS curves for the cuprate superconductors. However, as a newly proposed method, we would like to focus more on the method itself in this paper, i.e., to explain and attest the validity of the method, and meanwhile, to use some of the recently reported experimental tunneling data on the intrinsic Josephson junctions (IJJs) of $Bi_2Sr_2CaCu_2O_{8+\delta}$ (BSCCO) superconductors to show the capacity and the strength of the method. In particular, we discuss the criterion to determine the parameter α, which controls the competition between the squared error term and the information entropy term of the method. We suggest a stepwise process to adjust the mock function which would keep our solutions steering on the right track. We design two kinds of tests to examine the applicability of the inversion method.

As a preliminary study, we consider in this paper a sample doped close to the optimal doping with its doping concentration as $\delta = 0.19$ and the critical temperature $T_c = 89$ K (OP89 K) [11,12]. The DOSs at temperatures of $T = 4.2$ K, 45 K, 55 K, 95 K, and 130 K are successfully extracted from the corresponding experimentally measured $I(V)$ curves. Below T_c, it is observed that the energy gap decreases with increasing temperature, while above T_c, the gap actually survives. Considering the continuous evolution of the quasiparticle DOS versus the temperature, we may find that the present study has provided a fresh angle to tackle the pseudogap phenomenon in high-T_c superconductors.

The paper is organized as follows: In Sec. II we extend the maximum entropy approach to nonlinear systems and develop a scheme to extract the quasiparticle DOS directly from the experimentally measured $I(V)$ data. In Sec. III, we discuss the flexibility of the mock function and show the validity of our scheme with two examples. In Sec. IV, we apply the approach to the IJJ data performed on the optimally doped sample OP89K and present the obtained DOS curves. The energy gap persisting well above T_c is discussed. A summary is given in Sec. V.

II. MAXIMUM ENTROPY METHOD

A. Statement of the problem

The tunneling current as a function of voltage bias across the SIS tunneling junction can be often expressed as [13]

$$I(V_i) = \frac{1}{eR_N}\int_{-\infty}^{+\infty} N(\omega)N(\omega_i')[f(\omega) - f(\omega_i')]d\omega, \quad (1)$$

where $\omega_i' = \omega + eV_i$, $f(\omega)$ is the Fermi distribution function, and R_N is the resistance of the circuit. The index i denotes the ith measurement of tunneling current with the bias voltage V_i. In Eq. (1), $N(\omega)$ is the targeting quantity we are interested in. For those conventional SIS tunneling junctions sandwiched

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between two identical isotropic *s*-wave superconductors, Eq. (1) often works well in which case the $N(\omega)$ can be identified as the physical density of states. On the other hand, for the SIS intrinsic Josephson junctions growing on the crystal layers of the unconventional cuprate high-temperature superconductors, the $N(\omega)$ in Eq. (1) can be interpreted as the second-order azimuthal moment of the DOS, which can also be understood as a mean DOS averaging the angle-resolved DOS with a proper weight function (see Appendix for more details). However, as shown also in the Appendix, the curves of the DOS and those of its second-order moment are qualitatively similar to each other. We would like to keep the above understandings in mind and ignore formally the differences of the mentioned two cases such that we name $N(\omega)$ the "density of states" throughout this paper for simplicity.

Since the tunneling current $I(V)$ of Eq. (1) in principle can be measured precisely with advanced technology, can we extract the DOS $N(\omega)$ with enough precision through Eq. (1)? It is frequent to parametrize the DOS $N(\omega)$ with an *ad hoc* expression, and the parameters are determined by fitting Eq. (1) to the experimentally measured tunneling current $I_e(V_i)$ [14–20]. Obviously underlying physical assumptions have been already built in implicitly in such parametrization process. What we want is to have a model-independent way to extract the DOS $N(\omega)$ directly from the experimentally measured $I_e(V_i)$ data via Eq. (1) with as few assumptions as possible.

Equation (1) can be viewed as a functional response relation with $N(\omega)$ as its input and $I_c(V)$ its outcome, where index c means that the current $I_c(V)$ is calculated by Eq. (1). Our interest is to acquire the most probable DOS $N(\omega)$ which produces the outcome $I_c(V_i)$, in coincidence with the experimentally measured tunneling current $I_e(V_i)$ as precisely as possible.

B. The inversion method

For this purpose, we introduce the posterior probability $P[N(\omega)|I_e(V_i)]$, which is the conditional probability of $N(\omega)$ with the event $I_c(V_i)$ to have occurred as the measured $I_e(V_i)$. It is known [6–9] that $P[N(\omega)|I_e(V_i)] \propto P[I_e(V_i)|N(\omega)]P[N(\omega)]$, in which the prior probability $P[N(\omega)]$ is the probability that the DOS as its functional arguments takes the designated form $N(\omega)$, and $P[I_e(V_i)|N(\omega)]$, the so-called likelihood functional, is the conditional probability of producing the experimentally measured data $I_e(V_i)$ from a given function $N(\omega)$.

By applying the maximum entropy method, the posterior probability

$$P[N(\omega)|I_e(V_i)] \propto e^{-L} \tag{2}$$

with $L = \frac{1}{2}\chi^2 - \alpha S$, where the generalized Shannon-Jaynes entropy [4]

$$S = \int d\omega \left[N(\omega) - M(\omega) - N(\omega) \ln \frac{N(\omega)}{M(\omega)} \right] \tag{3}$$

is contributed by the prior probability $P[N(\omega)]$, and the sum of squared errors

$$\chi^2 = \sum_i [I_e(V_i) - I_c(V_i)]^2/\sigma_i^2 \tag{4}$$

is due to the likelihood functional $P[I_e(V_i)|N(\omega)]$. In the above expressions, σ_i is the i-dependent root-mean-square error and $M(\omega)$ is a model function, reflecting our best prior knowledge for $N(\omega)$, which is crucial for correctly extracting the DOS from the experimental $I(V)$ curve, and should respect the following constraints: (i) it is positive; (ii) it becomes 1 when $|\omega| \to \infty$. Then the most probable $N(\omega)$ can be obtained by optimizing the posterior probability $P[N(\omega)|I_e(V_i)]$ [Eqs. (2)–(4)] with respect to $N(\omega)$. Formally, this has the appearance of a conditional extrema problem: to maximize the entropy S subject to a constraint on χ^2 with a Lagrange multiplier $\frac{1}{\alpha}$.

Here we give a brief description of the numerical scheme adopted. First of all, we should discretize the continuous variable ω into a set of discrete numbers $\{\omega_k\}$. The densities of states defined on $\{\omega_k\}$ are denoted by $\{x_k\} \equiv \{N(\omega_k)\}$. Without loss of generality we consider the nth $\{x_k^{(n)}\}$ generated in the nth round of iteration. Since the intervals of the $\{\omega_k\}$ sequence usually may not be divided exactly by the values of the bias voltage eV_i, in order to carry out the integral over ω on the right-hand side of Eq. (1), we should construct by interpolation a continuous function $\{N^{(n)}(\omega)\}$ which is the continuation of the discrete set $\{x_k^{(n)}\}$. To make the evaluation more efficient, the obtained B-spline representation of the interpolated DOS should be further converted to a piecewise polynomial representation [21]. We may then calculate the current $I_c^{(n)}(V_i)$ for each V_i as well as the entropy $S^{(n)}$ with the density of states in Eqs. (1) and (3) substituted by the interpolated DOS $\{N^{(n)}(\omega)\}$, respectively. We may further introduce the $\chi^{(n)2}$ with the $I_c(V_i)$ in Eq. (4) replaced by $I_c^{(n)}(V_i)$. Finally, we obtain, for the nth round, $L^{(n)} = \frac{1}{2}\chi^{(n)2} - \alpha S^{(n)}$. We stress that, due to $\{N^{(n)}(\omega)\}$ being deduced from the sequence $\{x_k^{(n)}\}$ by interpolation, the $L^{(n)}$ is an implicit function of the $\{x_k^{(n)}\}$ sequence. Kept with such an understanding, $L^{(n)}$ can be written as $L^{(n)} \equiv L[x_1^{(n)}, x_2^{(n)} \cdots] \equiv L[\{x_k^{(n)}\}]$; then the convergence criterion of the iteration process is that the following inequality is satisfied:

$$\sqrt{\sum_k \left| \frac{\partial L^{(n)}}{\partial x_k^{(n)}} \right|^2} < \epsilon, \tag{5}$$

where the gradients are calculated by the finite-difference method and ϵ is the gradient tolerance.

If the convergence criterion cannot be satisfied at the nth round, we then have to get into the $(n+1)$th round of iteration and to generate the $\{x_k^{(n+1)}\}$ with the application of the quasi-Newton method [22].

C. The competition between χ^2 and S

There are two terms in the exponent of the posterior probability. The second is a term of information entropy S, which plays a role to make the DOS $N(\omega)$ to meet the mock function as much as possible, while the first term $\frac{1}{2}\chi^2$, a term of summation of the squared errors, tends to make the DOS $N(\omega)$-resulted tunneling current $I_c(V_i)$ to be close to the experimentally measured tunneling current $I_e(V_i)$. The parameter α plays a role to control the competition between these two terms. A big α will make the entropy term take over the squared error term and the resulting DOS will be close to the mock functions. If the parameter α becomes smaller and smaller, the first term will dominate over the second one and the extracted solutions will deviate from the mock function and give smaller χ^2.

It appears that with the $I_c(V_i)$ getting closer to the input $I_e(V_i)$, the resulting DOS $N(\omega)$ will meet the physical solution. However, since the optimization procedure referring to the first term is imposed directly on the $I_c(V_i)$ which is a complicated integral over the unknown function $N(\omega)$, such optimized $N(\omega)$ is not unique. In particular, fictitious solutions often occur with unphysical oscillations. On the other hand, the optimization with respect to the second term will not result in such fictitious oscillations due to the harmonic nature of the entropy. Although the mock function provides only partial information on the physical solutions, it is supposed to favor solutions lying along the physically right track.

Based upon the above considerations, it is desirable to choose α small enough to make $I_c(V_i)$ as close as possible to the input $I_e(V_i)$, and sufficiently large to carry the information of the mock function and suppress fictitious oscillations. A reasonable proposal for the choice of the value α is to request the order of magnitude of $[I_c(V_i) - I_e(V_i)]^2$ to be comparable with the given root-mean-square error of the ith measurement σ_i^2 or

$$\sum_{i=1}^{N_e} \frac{[I_c(V_i) - I_e(V_i)]^2}{\sigma_i^2} \sim N_e, \tag{6}$$

where N_e is the number of points of the experimental measurements.

We would like to suggest a scheme as a preliminary test of the inversion approach proposed above. We calculate the tunneling current $\tilde{I}_e(V_i)$ resulting from a known density of states $\tilde{N}(\omega)$. We may then pretend that the DOS $\tilde{N}(\omega)$ is unknown, and apply our scheme to Eq. (1) with the $I_e(V_i)$ identified as the input current $\tilde{I}_e(V_i)$ to extract the most probable DOS $N(\omega)$. A careful comparison between the obtained most probable DOS $N(\omega)$ and the known $\tilde{N}(\omega)$ would provide a test of our proposed approach.

In such a test scheme, because of the lack of mean-square errors, we set them simply to a constant σ^2. Then, as a result, the parameters α and σ^2 become no longer independent, which would lead a scaling relation as that, the increase of α can be compensated by the decrease of σ^2.

A detailed realization of this scheme together with the corresponding results is shown in the next section.

III. TESTS OF THE MAXIMUM ENTROPY METHOD

In the application of the maximum entropy method, the mock function $M(\omega)$, reflecting our best prior knowledge, plays an important role. In the process of extraction, we may adjust the mock function and hence, improve our results by iteratively inputting increasing amounts of prior knowledge. Generally, the extracted result with some mock function will suggest additional information which may help us tune the mock function in the next round calculation. Especially in our studies, if we know little about the quasiparticle density of states, we may use a flat model $m_1(\omega) = 1$ to extract a result $N_1(\omega)$ and then recalculate the density of states with a modified mock function $m_2(\omega)$ which includes some information of $N_1(\omega)$ (e.g., a peak). Such a stepwise way of successive improvement of the mock function as well as the corresponding resulting DOS curves is recommended, and meanwhile adopted in the following discussions.

In our calculations, to mimic the quasiparticle DOS of a superconductor, we take the mock function as the following: for $T < T_c$

$$M(\omega) = \begin{cases} \delta + (1-\delta)\left(\frac{\omega}{\omega_0}\right)^s, & \text{for } 0 \leqslant \omega \leqslant \omega_0, \\ 1, & \text{for } \omega > \omega_0, \end{cases} \tag{7}$$

with $s = 0$, 1, or 2. When $s = 0$, the mock function returns to the flat model. When $s = 1$ or 2 with $\delta = 0$, $(\frac{\omega}{\omega_0})^s$ resembles the low-energy behavior of the DOS for a d-wave or an s-wave superconductor. If the density of states at $\omega = 0$ is expected to be finite, we may set a finite δ. Moreover, ω_0 simulates the possibly existing energy gap, which can be estimated experimentally as the half of the first peak position of the experimental dI/dV curve, or theoretically as the peak position of the extracted DOS with the flat mock function; for $T > T_c$,

$$M(\omega) = 1 \tag{8}$$

for all energies.

The inversion calculation is performed in the domain $\omega \in [0,\omega_d]$ with ω_d much larger than the speculated gap so that $N(\omega)$ is assumed as $N(\omega) = 1$ when $\omega > \omega_d$. The domain is discretized inhomogeneously by N points $\{\omega_k\}$, $k = 1, 2, \ldots, N$, with more points distributed over an extension of the expected DOS peak. In our calculation, we take ω_d and N as large as $\omega_d = 170$ meV and $N = 70$, respectively. The root-mean-square error σ_i's are all set to be 0.1. In the calculation of $I(V)$ curve [Eq. (1)], an upper cutoff $\omega_c = 400$ meV is introduced. It is pointed out that our numerical results are not sensitive to these parameters.

A. Test with *s*-wave Dynes formula

A modified Bardeen-Cooper-Schrieffer (BCS) density of states first proposed by Dynes [23],

$$N_s(\omega) = \mathrm{Re}\left[\frac{\omega - i\Gamma}{\sqrt{(\omega - i\Gamma)^2 - \Delta^2}}\right], \tag{9}$$

is often used to mimic the tunneling current data, where Δ denotes the superconducting gap and Γ accounts for the lifetime broadening of the quasiparticle states.

At $T = 10$ K, 100 K, and 200 K with $(\Delta,\Gamma) = (36{,}5)$, $(33{,}8)$, $(23{,}10)$, respectively, we, on the one hand, calculate the Dynes DOSs designated as $\tilde{N}(\omega)$ and generate the $\tilde{I}_e(V_i)$ for $N_e = 75$ values of V_i via Eq. (1); on the other hand, we take the generated $\tilde{I}_e(V_i)$ as the "experimental data" and solve the DOS $N(\omega)$ with our numerical scheme. The comparisons between the designated and the extracted DOS curves are presented in Figs. 1 and 2.

At first, we take the mock function as $M(\omega) = 1$ and explain how to determine α. For a given α, we may extract a $N(\omega)$ by minimizing $L = \frac{1}{2}\chi^2 - \alpha S$ and then calculate the corresponding $\chi^2(\alpha)$ with the extracted DOS. As shown in

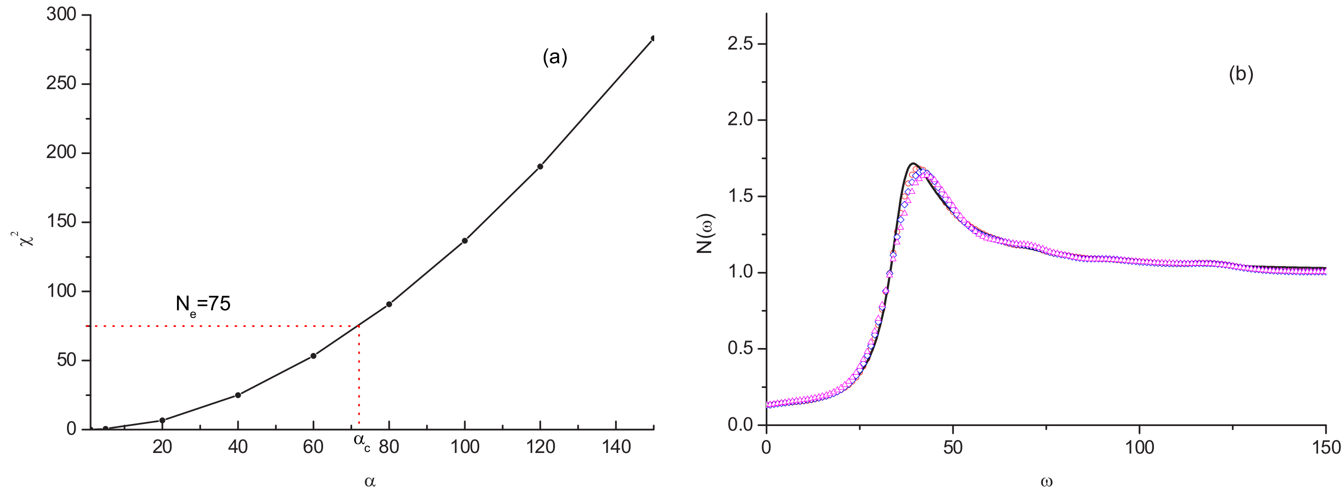

FIG. 1. (a) Variations of the calculated χ^2 with the extracted DOSs at different α's. α_c is determined with $\chi^2(\alpha_c) = N_e$. (b) Extracted $N(\omega)$ at $\alpha = 40$ (red circles), 80 (blue diamonds), and 150 (magenta triangles). The solid line denotes the DOS calculated with the Dynes formula [Eq. (9)] with $(\Delta,\Gamma) = (36,5)$. The temperature $T = 10$ K.

Fig. 1(a), α_c is then determined with $\chi^2(\alpha_c) = N_e$. In Fig. 1(b), we show the calculated $N(\omega)$'s for different α's. It is found that the extracted $N(\omega)$ changes slowly with the variation of α.

In Fig. 2, we explore the evolution of the DOSs with increasingly improved mock functions at different temperatures. The primary mock function is taken to be the flat model $M(\omega) = 1$. Such extracted $N(\omega)$ fits well with the inserted Dynes formula at low temperature ($T = 10$ K). At higher temperatures ($T = 100$ K, 200 K), the peak position deviates more and more. Considering the peak in the DOS curve, we then set a BCS s-wave-like mock function [Eq. (7) with $s = 2$ and $\delta = 0$] and recalculate the DOSs at $T = 10$ K, 100 K, and 200 K with $\omega_0 = 40$ meV, 39 meV, and 32 meV, respectively, where the ω_0 value is the corresponding DOS peak position extracted from the first-round calculation with the flat mock function. As shown in Fig. 2, the extracted results can now give the correct peak position. However, an unexpected small peak appears around 10 meV due to the mistaken assumption of zero DOS at zero energy. With the help of a finite δ and hence, a finite DOS at zero energy implemented in Eq. (7), we further improve the mock function and extract the DOSs most consistent with the inserted Dynes formula at low and high temperatures.

B. Test with a *d*-wave superconductor

Another interesting example of the suggested test scheme is the SIS tunneling current in the d-wave BCS theory, where the DOS $\tilde{N}(\omega)$ is known as [24]

$$\tilde{N}(\omega)/N_0 = \begin{cases} \frac{2}{\pi} x K(x), & \text{for } x \leqslant 1, \\ \frac{2}{\pi} K(x^{-1}), & \text{for } x > 1, \end{cases} \tag{10}$$

in which $x = \omega/\Delta$ with Δ the superconducting energy gap and $K(x)$ the complete elliptic integral.

Differently from the phenomenological Dynes formula, the DOS now vanishes at zero energy. More interestingly, the gap is a universal function of the temperature for a BCS superconductor if it is scaled by the gap value measured at zero temperature and by the critical temperature T_c, so the DOS curves calculated at a single temperature characterize the full temperature dependence. However, in the maximum entropy inversion approach engaged here, such scaling relation could break down due to the introduction of the mock function

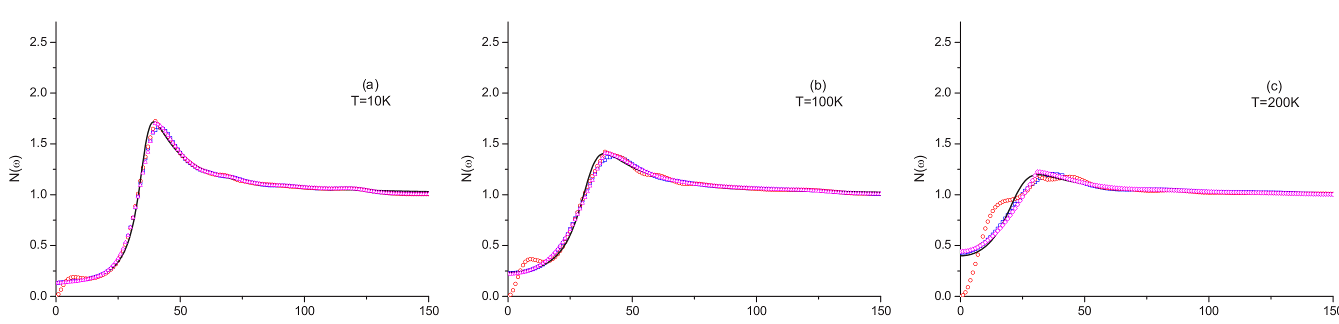

FIG. 2. Extracted DOSs at temperatures (a) $T = 10$ K, (b) $T = 100$ K, and (c) $T = 200$ K with three different mock functions: (i) flat mock function $M(\omega) = 1$ (blue squares), (ii) s-wave-like mock function Eq. (7) with $s = 2$ and $\delta = 0$ (red circles), and (iii) mixed mock function Eq. (7) with $s = 2$ and a finite δ of 0.15, 0.24, and 0.4 at temperature of 10 K, 100 K, and 200 K, respectively (magenta triangles). The solid line in (a)–(c) denotes the DOS of the Dynes formula [Eq. (9)] calculated with $(\Delta,\Gamma) = (36,5)$ (a), $(33,8)$ (b), and $(23,10)$ (c), respectively.

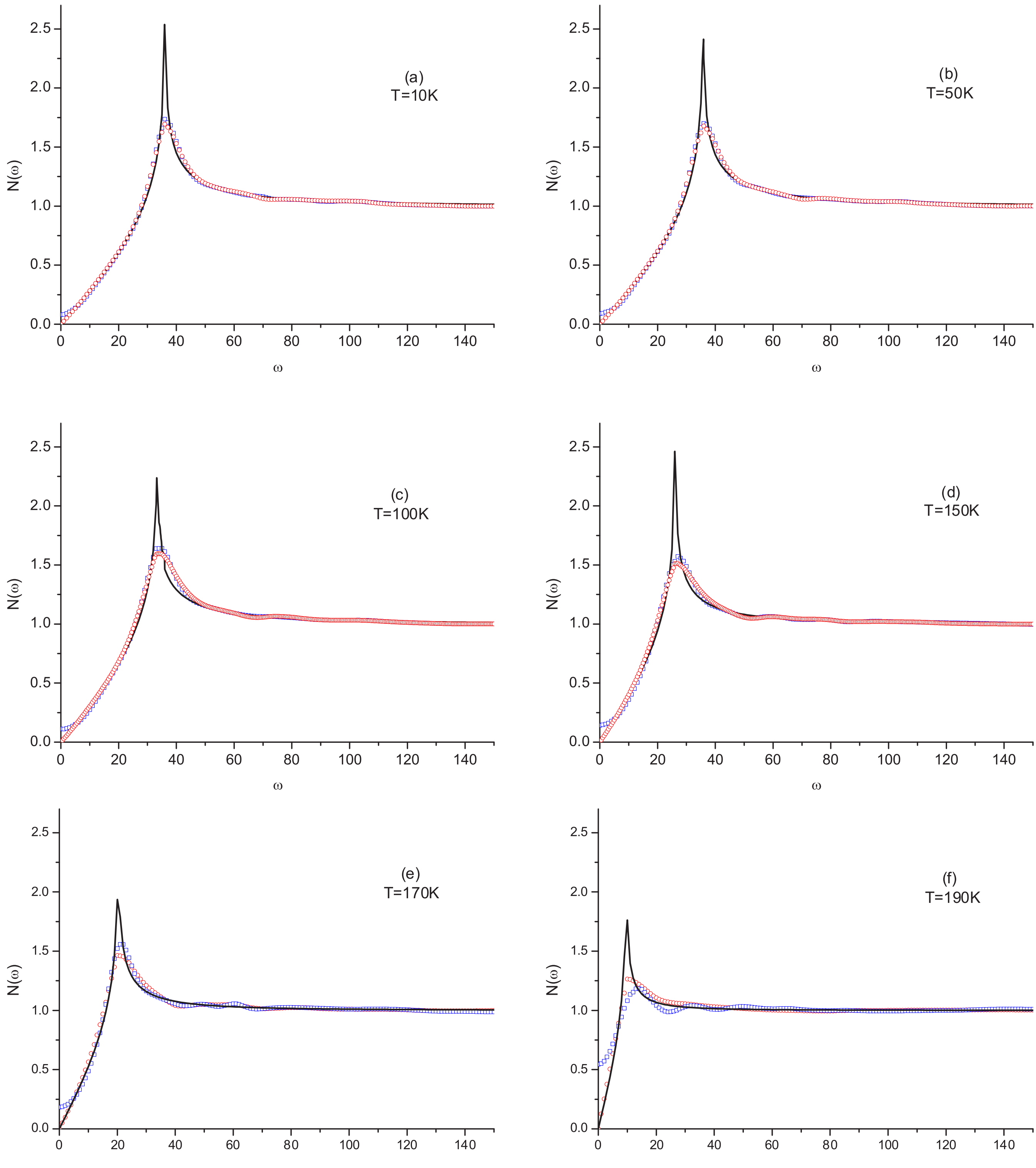

FIG. 3. Extracted DOSs at various temperatures from $T = 10$ K to $T = 190$ K with the mock function of (1) $M(\omega) = 1$ (blue squares) and (2) Eq. (7) with $s = 1$, $\delta = 0$, and $\omega_0 = 36$ meV (a), 35 meV (b), 33 meV (c), 26 meV (d), 20 meV (e), and 10 meV (f) (red circles). The solid line in (a)–(f) denotes the DOS of the d-wave superconductor [Eq. (10)] calculated at the given temperature.

[Eqs. (7) and (8)]. In particular, it is desirable to see whether our approach can still produce meaningful results when the gap shrinks with increasing temperature.

The tests are performed with two different mock functions at $T = 10$ K, 50 K, 100 K, 150 K, 170 K, and 190 K, with the gap value Δ at $T = 0$ K chosen to be 36 meV. The comparisons between the extracted $N(\omega)$'s and $\tilde{N}(\omega)$ are shown in Fig. 3.

With the flat mock function $M(\omega) = 1$, the extracted $N(\omega)$'s reproduce the peak structure and fit the inserted d-wave DOS

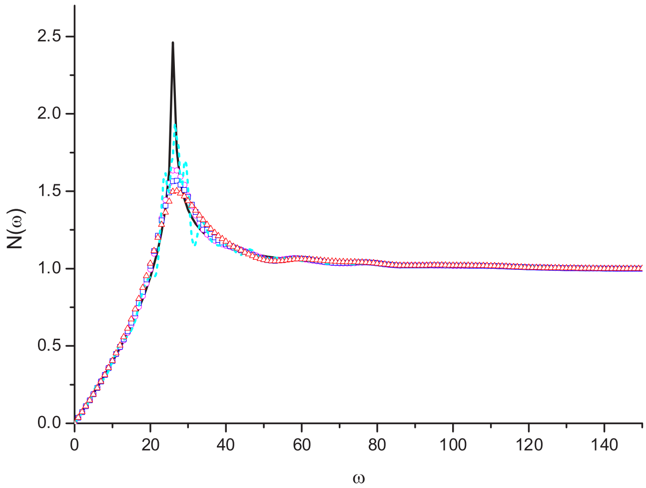

FIG. 4. Extracted DOSs at $T = 150$ K with $\alpha = 1$ (dashed line), 50 (red circles), 100 (blue squares), and 200 (magenta triangles). The solid line denotes the d-wave DOS [Eq. (10)] at $T = 150$ K.

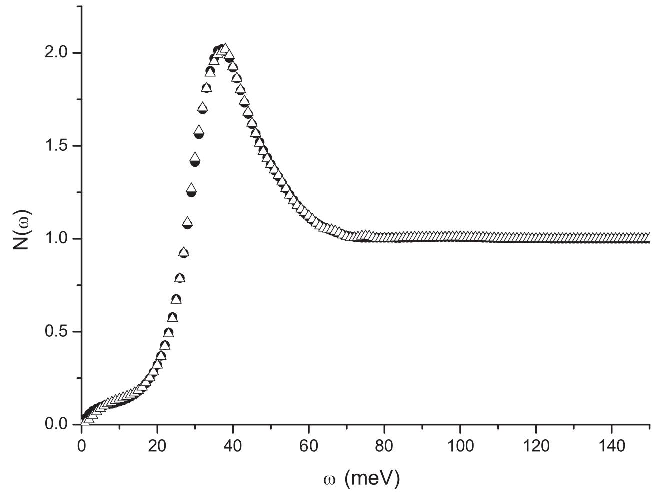

FIG. 5. Extracted DOSs from the $I(V)$ curve measured at $T = 4.2$ K with $\alpha = 50$, $\omega_0 = 30$ meV, $s = 1$ (filled circles), and $s = 2$ (open triangles).

$\tilde{N}(\omega)$ quite well at low and moderate temperatures except a finite but tiny value at zero energy. At high temperatures ($T = 170$ K, 190 K), the deviations at low energies become large and especially, some oscillations appear on the right of the peak.

Considering the peak structure, we then use a d-wave-like mock function as described in Eq. (7) with $s = 1$, $\delta = 0$, and $\omega_0 = 36$ meV ($T = 10$ K), 35 meV ($T = 50$ K), 33 meV ($T = 100$ K), 26 meV ($T = 150$ K), 20 meV ($T = 170$ K), and 10 meV ($T = 190$ K). Now, the results are improved much; i.e., the extracted $N(\omega)$'s coincide well with the inserted $\tilde{N}(\omega)$'s at each temperature and the oscillations diminish greatly.

As discussed in Sec. II, spurious oscillations may enter into our results. To get more insights, in Fig. 4, we show the extracted DOSs with four different α's at $T = 150$ K. The oscillations are easily seen at small α and are depressed quickly at large α. Generally, we may improve our results with a higher accuracy, and more effectively, with a better mock function containing more information of our target quantity.

From Figs. 1, 2, 3, and 4, we can see that the maximum entropy method is effective in extracting the DOS from the experimental data. The solutions are quite stable and can be ameliorated by an increasingly improved mock function. In the process of extraction, it is suggested to provide our best prior knowledge and speculate a suitable mock function as close as possible to the real case.

IV. PRELIMINARY APPLICATION TO $Bi_2Sr_2CaCu_2O_{8+\delta}$

Now we apply our approach to the recently reported $I(V)$ curve, which is a precise measurement performed on intrinsic Josephson junctions (IJJs) of $Bi_2Sr_2CaCu_2O_{8+\delta}$ superconductors with the CuO_2 double layers as superconducting electrodes and BiO/SrO interlayers as the tunnel barrier [11,12]. In our process of extraction, the mock function is chosen as in Eqs. (7) and (8) with $\delta = 0$.

It is well established that the superconducting gap in high-T_c superconductors has a dominant d-wave symmetry across the entire phase diagram, although a smaller s component cannot be ruled out [25]. The pairing symmetry may also depend on inhomogeneities, doping, and impurities. For a d-wave superconductor, the quasiparticle density of states has a logarithmic peak at $\omega = \Delta_{sc}$ and increases linearly with ω for small ω/Δ_{sc}. In a pilot calculation, we have tested the DOS inversion calculation for a specified $I(V)$ curve measured at $T = 4.2$ K, with $s = 1$ and 2, yet $\omega_0 = 30$ meV being kept fixed. As shown in Fig. 5, the two calculated DOS curves coincide with each other pretty well except a little difference at small ω, which will not affect our main conclusions. Although we have no preference for the parameters $s = 1$ or 2, we will set $s = 1$ in the following calculations.

Another parameter ω_0 in Eq. (7) is estimated as half of the first peak position of the experimental dI/dV curve. At $T = 4.2$ K, 45 K, and 55 K, the obtained ω_0 equals 37 meV, 36 meV, and 35 meV, respectively. These values are consistent with the peak positions of the extracted DOSs with the flat mock function. For brevity, we do not show these curves here.

With the mock function as well as the parameters discussed above, we extract $N(\omega)$'s at temperatures $T = 4.2$ K, 45 K, 55 K, 95 K, and 130 K, as shown in Fig. 6. Below T_c, a sharp peak structure, corresponding to an energy gap, is found in the $N(\omega)$ curve. This energy gap decreases with increasing temperature. Interestingly, a wide, but still well-shaped, peak can be also observed above T_c, which indicates that a kind of energy gap is opened when the superconductivity disappears. We emphasize that the result of a finite gap surviving at temperature $T > T_c$ is obtained without any *a priori* input through the mock function [Eq. (8)]. Although the pseudogap above T_c has been observed in various experiments and has been extensively discussed for many years (see, for example, Refs. [2] and [3]), its origin and its relation to the mechanism of high-T_c superconductivity are still unclear. Our study provides an angle to investigate this phenomenon, exhibiting its evolution continuously from below T_c to high above it.

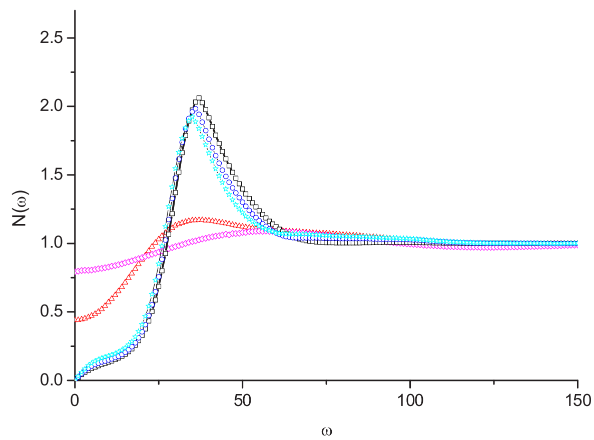

FIG. 6. Extracted DOSs in OP89K at temperatures $T = 4.2$ K (black squares), 45 K (blue circles), 55 K (cyan stars), 95 K (red triangles), and 130 K (magenta diamonds).

More results, including the extracted $N(\omega)$'s around T_c and those DOS curves obtained in the underdoped and overdoped samples, will be presented elsewhere, together with a discussion on the complicated phase diagram of high-T_c superconductors [26].

V. SUMMARY

In this paper, we propose to extract the quasiparticle density of states of a superconductor directly from the experimentally measured superconductor-insulator-superconductor (SIS) tunneling data by applying the maximum entropy method to the tunneling current expression Eq. (1). Various ingredients of the proposed method have been carefully examined, including the meaning of the target function $N(\omega)$ in Eq. (1), the role and the designation of the input parameters α, as well as the mock function. The method has the advantage of being independent of microscopic/theoretical models for the superconductors under investigation. The validity of the developed scheme is shown by two tests for systems with known DOSs, of which one is an s-wave superconductor with its DOS given by the Dynes formula and the other is the BCS d-wave superconductor with the known quasiparticle DOS given by Won and Maki [24]. The resulting numerical solutions are stable with minimum *a priori* physical assumptions and can be improved by successive refinements of the mock function.

In a preliminary application to the cuprate superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$ (OP89K), we obtain a series of DOS curves at temperatures $T = 4.2$ K, 45 K, 55 K, 95 K, and 130 K. Below T_c, the energy gap decreases with increasing temperature. Above T_c, the energy gap survives when superconductivity disappears. Imaged by the continuous evolution of the quasiparticle DOS versus temperature, the energy gap inferred from these calculated DOS curves evolves smoothly from the temperature below T_c to that above T_c, which may provide a fresh angle to tackle the pseudogap phenomenon in high-T_c superconductors.

Our method might be an interesting and possibly useful tool for future applications in various fields, particularly, for the study of the nature of cuprate high-T_c superconductivity.

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APPENDIX

It is known that the tunneling current as a function of voltage bias across the SIS tunneling junction can be expressed as [27]

$$I(eV) = 2e\sum_{\vec{k},\vec{p}}|T_{\vec{k},\vec{p}}|^2\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}A^{(R)}(\vec{k},\omega)$$
$$\times A^{(L)}(\vec{p},\omega+eV)[f(\omega)-f(\omega+eV)], \quad \text{(A1)}$$

where $A^{(R)}(\vec{k},\omega)$ and $A^{(L)}(\vec{p},\omega+eV)$ are the spectral functions for the right- and left-hand side superconductors of the tunneling junction, respectively. For a conventional isotropic superconductor sandwiched with a tunneling junction, the momentum dependence of tunneling matrix elements can be often ignored, i.e.,

$$|T_{\vec{k},\vec{p}}|^2 \sim |T|^2; \quad \text{(A2)}$$

then the tunneling current Eq. (A1) can be simplified to the form Eq. (1), in which the coefficient

$$\frac{1}{eR_N} = 4\pi e|T|^2, \quad \text{(A3)}$$

and

$$N(\omega) = \frac{1}{2\pi}\sum_{\vec{k}}A(\vec{k},\omega) \quad \text{(A4)}$$

is the physical DOS [27]. For the layered high-T_c superconductor samples such as BSCCO, the intrinsic SIS junctions are grown on the crystal layers. The tunneling quasiparticle moves along the C-axis direction perpendicular to the CuO planes, with a velocity estimated to be proportional to $\cos^2(2\varphi)$, where φ is the in-plane angle of the particle momentum. Following Bardeen [28] and Harrison [29], the tunneling matrix element is proportional to the velocity of the quasiparticle, which results in [30]

$$|T_{\vec{k},\vec{p}}|^2 \sim 4|T_0|^2\cos^2(2\varphi_L)\cos^2(2\varphi_R). \quad \text{(A5)}$$

Substituting expression Eq. (A5) into Eq. (A1), it can be verified straightforwardly that the tunneling current can be put into a form again coincident with Eq. (1), yet the $N(\omega)$ is no longer DOS, and becomes

$$N(\omega) = \frac{1}{2\pi}\sum_{\vec{k}}2\cos^2(2\varphi)A(\vec{k},\omega) \quad \text{(A6)}$$

as the second-order azimuthal moment of the DOS.

We may introduce

$$N_d(\omega,\varphi) = \sum_{\vec{k}}\delta(\varphi-\varphi_{\hat{k}})A(\vec{k},\omega) \quad \text{(A7)}$$

with $\vec{k} = (k_x,k_y) = (k\cos\varphi_{\hat{k}},k\sin\varphi_{\hat{k}})$, which has the physical meaning as the angle-resolved DOS of the quasiparticles.

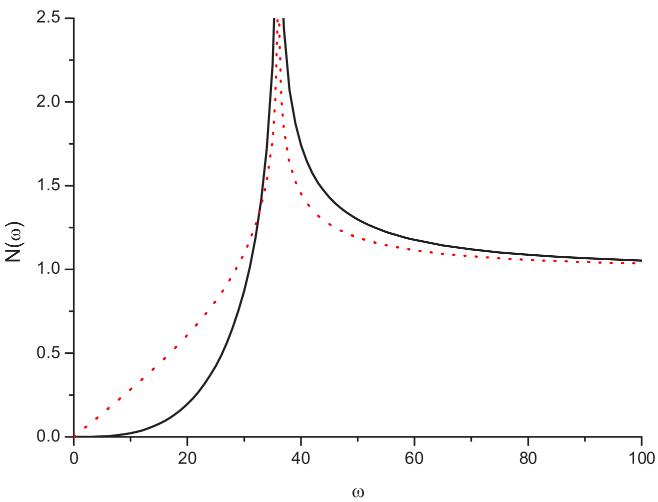

FIG. 7. Calculated DOS $N(\omega)$ from Eqs. (A8) and (A9) with $m = 0$ (dotted line) and $m = 1$ (solid line), respectively. $\Delta = 36$ meV.

Then, both Eqs. (A4) and (A6) can be expressed as

$$N(\omega) = \frac{2^m}{2\pi}\int_0^{2\pi} \cos^{2m}(2\varphi) N_d(\omega,\varphi) d\varphi \tag{A8}$$

with $m = 0$ and 1, respectively, where a unified boundary condition $\lim_{\omega\to\infty} N(\omega) = 1$ is invoked. Equation (A8) can also be viewed as a mean DOS averaging the angle-resolved DOS over the azimuthal angle φ with a weight function $2^m \cos^{2m}(2\varphi)$ [16–19].

For comparison of the two cases, we calculate numerically $N(\omega)$ curves following Eq. (A8) with the application of d-wave BCS theory as that

$$N_d(\omega,\varphi) = \mathrm{Re}\left[\frac{\omega}{\sqrt{\omega^2 - \Delta^2\cos^2 2\varphi}}\right], \tag{A9}$$

where Δ is chosen to be 36 meV. As shown in Fig. 7, the DOS curves with $m = 0$ and 1 exhibit similar shape with a peak at the same position. The discrepancy between them becomes apparent in the low-energy region, where the curve of $m = 0$ approaches zero linearly while that of $m = 1$ drops down to zero much more quickly.

We note that in the case in which the tunneling is specular for a planar junction, the two summations $\sum_{\vec{k}}$ and $\sum_{\vec{p}}$ in Eq. (A1) become no longer independent of each other due to the conservation of in-plane momentum. Then, Eq. (1) breaks down [29].

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