Holographic maps of quasiparticle interference

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The analysis of Fourier-transformed scanning tunnelling microscopy images with subatomic resolution is a common tool for studying the properties of quasiparticle excitations in strongly correlated materials. Although Fourier amplitudes are generally complex valued, earlier analysis primarily focused on their absolute values. Their complex phases were often deemed random, and thus irrelevant, due to the unknown positions of the impurities in the sample. Here we show how to factor out these random phases by analysing overlaps between Fourier amplitudes that differ by reciprocal lattice vectors. The resulting holographic maps provide important and previously unknown information about the electronic structures. When applied to superconducting cuprates, our method solves a long-standing puzzle of the dichotomy between equivalent wavevectors. We show that d-wave Wannier functions of the conduction band provide a natural explanation for experimental results that were interpreted as evidence for competing unconventional charge modulations. Our work opens a new pathway to identify the nature of electronic states in scanning tunnelling microscopy.

Fourier-transformed scanning tunnelling spectroscopy (FT-STS) is a powerful technique based on Fourier transforming the local density of states measured by a scanning tunnelling microscope (STM). The resulting maps deliver information about the scattering of quasiparticles in the conduction band, and can be employed to reconstruct their dispersion relation. In the past two decades, this technique has found important applications in the study of high-temperature superconductors, where the nature of the band that is responsible for superconductivity is still debated.

Properties of the holographic maps

FT-STS maps are obtained by the two-dimensional Fourier transform of the differential tunnelling conductance, \( g(r,V) = \frac{dI}{dV} \), measured in STM experiments. The g maps defined by \( g(q,V) = \int d^2r e^{iqr} g(r,V) \) are generically complex valued. In disordered samples their phase depends on the position of the scatterers. (This is a simple consequence of the fundamental property of Fourier transformations, stating that a shift in real space corresponds to a phase rotation in momentum space.) If a single impurity is present, then this phase is given by \( e^{i\pi r_0} \), where \( r_0 \) is the position of the impurity, and can be factored out by choosing the axis origin in correspondence to the centre of the impurity (\( r_0 = 0 \)). In contrast, when analysing doped materials, several scatterers should be taken into account. In this case, the phase of the g map depends on the random configuration of the disorder and is therefore often assumed to provide little information about the material. One possible solution is to consider the auto-correlations of the STM signal in real space, which imply an ensemble average over the position of the impurities. This method was employed, for example, by ref. 36, to study electronic states close to the superconducting–insulator phase transition.
Here we instead propose to work in momentum space and to consider the overlaps of $g$ maps shifted by a generic reciprocal lattice vector $G$. Specifically, we define the holographic maps

$$h_G(q, V) = g(q, V) g^* (q + G, V) \quad (1)$$

As will be shown below, under realistic assumptions both the absolute value and the phase of $h_G(q, V)$ do not depend on the random position of the impurities on the lattice. In the case of $G = 0$, equation (1) simply reduces to $|g(q, V)|^2$, confirming the known fact that the absolute value of $g$ maps does not depend on the position of the impurities. For all other Brillouin vectors $G \neq 0$, equation (1) delivers additional information that was previously hidden in the $g$ maps.

To clarify the effects of disorder on Fourier-transformed maps, it is useful to consider $N$ identical randomly distributed weak scatterers on a lattice. To the lowest order in perturbation theory, the resulting $g$ map is $g(q, V) = \sum_{i} e^{i q \cdot r_i} g_{0}(q, V)$, where $r_i$ are the positions of the scatterers and $g_0(q, V)$ is the map generated by a single scatterer. Performing an ensemble average over the position of the scatterers we obtain $\langle g(q, V) \rangle = 0$ and $\langle |g(q, V)|^2 \rangle = \sum_{i,j} e^{i q \cdot (r_i - r_j)} \langle g_{0}(q, V) \rangle^2 = N \langle g_{0}(q, V) \rangle^2$, where $N$ is the number of impurities and we used $\delta_{r_i r_j} = \delta_{ij}$. As expected, we find that, although $g(q, V)$ averages to zero, its absolute value remains finite. In principle, a similar argument would suggest that ensemble-averaged $h$ maps should vanish as well. However, this is not the case if all the scatterers are physically equivalent, such as in the case of identical chemical substitutions, all located in the same positions of the unit cell. For this ensemble $G \cdot r = \phi_0$ is constant and

$$h_G(q, \omega) = \sum_{i} e^{i q \cdot r_i - \omega \varepsilon_i} g_{0}(q, V) g^*_0 (q + G, V)$$

$$= Ne^{-\omega \phi_0} g_0(q, V) g^*_0 (q + G, V) \quad (2)$$

We find that $h$ maps are invariant under ensemble average, up to an overall wavevector-independent phase factor, $e^{-\omega \phi_0}$. (As explained in the Methods, this phase factor can be removed by an appropriate choice of the origin of the Fourier transform.) In actual materials, several types of scatterers are often present—for example, as a consequence of distinct dopants, oxygen vacancies, or pinned vortices. For simplicity in this paper we focus on the case of one dominant type of scatterer, relevant to superconducting cuprates\textsuperscript{30,34}. Extension to several sources of disorder is straightforward.

**Experimental measurement of $h$ maps**

To demonstrate the usefulness of the present approach, we consider the specific case of Bi$_2$Sr$_2$La$_{0.5}$CuO$_{4.5}$ (Bi2201). Experimentally measured $h$ maps of this material are shown in Fig. 2. (See Methods for details and Supplementary Section 2 for a second sample of the same material, at a different doping.) Figure 2a simply represents the square of the absolute value of the $g$ map. It displays a broad peak around $q = 0$, and four star-shaped patterns at the four Bragg peaks $G_{r} = (\pm 1, 0)$ and $(0, \pm 1)$. For brevity we express all wavevectors in units of $2\pi/a$. Each of these patterns include four distinct satellites, located respectively at $q_i = G_i \pm (\delta, 0)$ and $G_i \pm (0, \delta)$, where $\delta = 0.2$ is material and doping dependent\textsuperscript{35}. A closer inspection of the data\textsuperscript{23} reveals pronounced shoulders in the central Brillouin zone as well, at wavevectors $q_{i}^{*} = (\pm \delta, 0)$ and $(0, \pm \delta)$. These peaks are commonly interpreted\textsuperscript{37-41} as evidence of a static (chequerboard?) modulation with wavevector $\delta$. The same type of incommensurate short-range ordered (SRO) order was observed in X-ray scattering experiments\textsuperscript{32,43} and is currently the focus of an intense theoretical and experimental investigation\textsuperscript{44-47}. For a long time, the observed difference between the visibility of the peaks at $q_{i}^{*}$ and $q_{i}^{*}$ has been regarded as an unsolved puzzle\textsuperscript{24-25}. To better understand the nature of these peaks, ref. 26 introduced a real-space masking procedure, which revealed that the $q_{i}^{*}$ peaks that differ by the inverse lattice vector $(1, 1)$

![Image](https://example.com/NaturePhysics_Figure1.png)

**Figure 1** Main steps and notations involved in the creation of holographic maps. $h$ maps are generated independently from the experimental measurements and from a phenomenological lattice model (see text for details). The comparison between the $h$ maps obtained by the two methods is used to deduce the shape of the Wannier function.

![Image](https://example.com/NaturePhysics_Figure2.png)

**Figure 2** Experimentally measured holographic maps for an optimally doped sample of Bi2201 with critical temperature $T_c = 35$ K, at voltage $V = 40$ meV. a. When $G = (0,0)$, the $h$ map simply corresponds to the square of the absolute value of the FT-STS map. b, c, For $G = (1,0) \times (2\pi/a)$ and $G = (0,1) \times (2\pi/a)$ (c), the $h$ map displays star-shaped patterns with d-wave symmetry, which demonstrate the necessity of non-trivial Wannier functions to interpret the data (see text for details). d, For $G = (1,1) \times (2\pi/a)$, the $h$ map is negative, in agreement with the $d$-form factor proposed by refs 26–28,54–56. Grey areas refer to wavevectors that are beyond the present experimental resolution.
Figure 3 | Schematic and theoretical $g$ maps. a, Schematic plot of the $g$ map of the $d$-form factor proposed by ref 26–28,54–56, implying that $q_1^+$ peaks that differ by $(1,1)$ have opposite signs. This finding is consistent with the present analysis, which additionally shows a coherence between the $q_1^+$ and $q_2^+$ peaks that differ by $(1,0)$. b, Schematic plot of the $g$ map deduced from the present analysis, characterized by a global $s$-wave rotational symmetry. c, Numerically computed $g$ map at $V = 40 \text{ meV}$, showing the same symmetry as b. These $g$ maps assume an isolated scatterer at the axis origin and cannot be directly compared to experiments due to the random position of the impurities in actual experimental samples. However, the correctness of our interpretation is demonstrated by the symmetry of the corresponding holographic maps.

**Figure 4** Theoretical holographic maps generated from the $g$ map depicted in Fig. 3c. a, $G = (0,0)$. b, $G = (1,0)$. c, $G = (0,1)$. d, $G = (1,1)$. All four $h$ maps precisely reproduce the experimental results presented in Fig. 2, including, in particular, the different symmetries and visibilities of the $q_1^+$ and $q_2^+$ peaks.

have opposite signs (see Fig. 3a and Supplementary Section 1 for details). This configuration is termed the $d$-form factor and had been theoretically predicted by Sachdev and collaborators27,28. The negative sign between $q_1^+$ peaks is here confirmed by the negative sign of the $h_{(1,1)}$ map shown in Fig. 2d. As we explain below, this effect arises naturally, due to the non-trivial Wannier function of cuprates.

The $h$ maps allow us to extract additional phase information and to determine the phase coherence between the peaks at $q_1^+$ and $q_2^+$ as well. These peaks differ by $(1,0)$ and their overlap is encoded in $h_{(1,0)}$, reproduced in Fig. 2b. As expected, this map shows two identical patterns, respectively centred around $(0,0)$ and $(1,0)$. Each pattern includes four satellites, which originate from the overlaps between the four inequivalent $q_1^+$ peaks and their corresponding $q_2^+$ peaks that differ by $(1,0)$ wavevectors. Remarkably, we find that these overlap patterns have a local $d$-wave symmetry. This finding indicates that either the $q_1^+$ pattern has a $s$-wave symmetry and each of the $q_2^+$ patterns has a local $d$-wave symmetry, or vice versa. The former interpretation is consistent with the observed intensity of the FT-STS signal and explains the different visibility of the peaks. Because the $g$ map in the central Brillouin zone is $s$-wave symmetric, its intensity is roughly rotationally invariant and partially hides the $q_2^+$ peaks. In contrast, the $g$ map in the first Brillouin zone has a local $d$-wave symmetry and vanishes along the two diagonals, accentuating the four $q_1^+$ peaks. Combining this information with the above-mentioned $d$-form factor, we obtain the $g$ map schematically shown in Fig. 3b. Remarkably, this map has a global $s$-wave symmetry (that is, it is invariant under rotations of $90^\circ$).

**Theoretical calculation of $h$ maps**

Wannier functions offer a natural explanation for the inequivalence of FT-STS maps in distinct Brillouin zones, and in particular for the dichotomy between $q_1^+$ and $q_2^+$. Wannier functions were used, for example, in ref. 48, to interpret non-resonant inelastic X-ray scattering (RIXS) experiments. The effects of Wannier functions on $g$ maps were first theoretically considered by ref. 2, and later applied to the study of actual materials29–50. In Supplementary Section 3 we employ the Bloch theorem to show that

$$g(q, V) = \sum_k W(k) W(k + q) G_{k, k}(V)$$

Here the reduced wavevector $\tilde{k} = k \mod G$ is restricted to the first Brillouin zone, while the sum over $k$ runs over all wavevectors; $G_{k, k}(V)$ is the retarded Green's function of the conduction band, and corresponds to the scattering amplitude of quasiparticles from momentum $k$ to $\tilde{k}$.

To generate theoretical FT-STM maps we need to specify a lattice model for $G_{k, k}(V)$. Following our earlier findings29,30, we claim that the chequerboard-type short-range order observed in STM experiments simply corresponds to Friedel oscillations around local impurities, rather than to a competing charge-density-wave (CDW) order. We specifically consider the scattering of quasiparticles with finite lifetime from local modulations of the pairing gap. This type of modulation can be induced by static disorder, or in the presence of an applied magnetic field, by the core of a pinned vortex29,51,52. The resulting $g$ map is presented in Fig. 3c (see Methods for details of the calculation); its structure coincides with the schematic plot inferred from the experiments in Fig. 3b. As explained above, in actual experiments, $g$ maps are multiplied by the random phase $e^{i\phi}$, which can be factored out by computing the $h$ maps. The results of our theoretical calculations are shown in Fig. 4, and accurately reproduce all the details of the experimental findings (Fig. 2). In particular, our theoretical calculations account for the above-mentioned local and global symmetries of the $h$ maps and...
for the dichotomy between the weaker features at \( q_x^a \) and the sharper peaks at \( q_y^a \).

The theoretical predictions shown in Fig. 4 were obtained using a Wannier function with \( d \)-wave symmetry and Gaussian envelope

\[
W(x) = (x^2 - y^2)e^{-\frac{(x^2 + y^2)}{2\sigma^2}},
\]

where \( \sigma \) sets the global size of the Wannier function. In our calculations this parameter was used as the only free fitting parameter. The best agreement between theory and experiment was obtained for \( \sigma \approx 0.3a \), where \( a \) is the unit cell length, leading to the Wannier function plotted in Fig. 5a. Interestingly, this wavefunction is significantly narrower than the one predicted by the first-principles calculations of ref. 50, for which \( \sigma \approx 0.7a \). An intuitive argument for the relation between this Wannier function and the resulting FT-STS maps is provided in Supplementary Section 4. To further highlight the fundamental role of the Wannier function on the FT-STS maps, in Supplementary Figs 3–6 we present calculations for alternative functions with different sizes and symmetries. In particular, we consider two families of extended Wannier functions, respectively proportional to \( x^2 + y^2 \) and \( |x^2 - y^2| \), (see Fig. 4b,c). While both functions have the same symmetry under rotations by 90°, the resulting \( h \) maps are very different, and only the latter is consistent with the experimental results. On the other hand, we observe that the \( h \) maps generated by \( W \sim x^2 - y^2 \) and \( W \sim |x^2 - y^2| \) are very similar. In general, we observe that FT-STS maps are more strongly affected by the shape of the absolute value of the Wannier function than by the symmetry of its phase. Note that, in our model, FT-STS maps are always \( s \)-wave symmetric, irrespective of the symmetry of the Wannier function. Therefore, to discern between \( d \)-wave \((W \sim x^2 - y^2)\) and \( s \)-wave \((W \sim |x^2 - y^2|)\) Wannier functions it is necessary to invoke additional arguments, such as the physical requirement of the Wannier function to be analytic (to avoid large kinetic-energy costs), or reasoning based on the relevant orbital (see, for example, ref. 53). In our case, both arguments support the \( d \)-wave Wannier function of equation (4) and Fig. 5a.

The present analysis can be readily applied to existing STM measurements of other non-conventional materials. Specifically, FT-STS maps of iron-based superconductors show four sets of inequivalent Brillouin zones, with distinct shapes. The analysis of holographic maps of these materials may help to solve long-standing debates about the nature of their conduction bands (see ref. 15 and references therein).
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Author contributions
All three authors equally contributed to the present study. E.G.D.T., Y.H. and E.D. conceived the idea of holographic maps and demonstrated their relation to the Wannier functions, E.G.D.T. and Y.H. analysed the experimental data, E.G.D.T. performed the numerical calculations, E.G.D.T. and E.D. wrote the manuscript.

Additional information
Supplementary information is available in the online version of the paper. Reprints and permissions information is available online at www.nature.com/reprints. Correspondence and requests for materials should be addressed to E.G.D.T.

Competing financial interests
The authors declare no competing financial interests.
Methods

The experimental holographic maps shown in Fig. 2 are based on STM measurements of an optimally doped sample of Bi2201 ($T_c = 35$ K) performed by the Hudson group. Each map includes approximately $400 \times 400$ points in real space, corresponding to a total surface of approximately $200 \times 200$ unit cells, or (0.1 nm)$^2$. Some real-space differential conductivity maps of these samples were reported in Figs 1(c) and 2(a–c) of ref. 23. Following ref. 26 we focus on the signal at a voltage $V = 40$ meV that is larger than the average pairing gap $\Delta_0 \approx 20$ meV (ref. 29). See also Supplementary Section 5 for some considerations concerning the voltage dependence of the holographic maps.

The analysis of the experimental data consists of two main steps: The differential conductivity at a fixed voltage is Fourier transformed to generate a $g$ map. As explained in the main text, these maps are characterized by a random wavevector-dependent phase, related to the unknown positions of the impurities. Next, the $h$ maps are computed by multiplying shifted $g$ maps with the complex conjugate of the unshifted map. The resulting $h$ maps are complex valued, and a direct comparison with the theoretical predictions requires the choice of a specific complex quadrature, equivalent to a specific choice of the axis origin of the Fourier transform: under a translation of the axis origin by $(x, y)$, the holographic maps are transformed as $h_{1,0} \rightarrow h_{1,0} e^{i2\pi x}$, $h_{0,1} \rightarrow h_{0,1} e^{i2\pi y}$, and $h_{1,1} \rightarrow h_{1,1} e^{i(2\pi x + 2\pi y)}$. In Fig. 4 we have chosen the pair of $\delta x$ and $\delta y$ that maximize the real component of the $h$ maps and plotted this component only. (See also Supplementary Section 6 for details.)

In our theoretical calculations we computed the scattering amplitude $G_{k,k'}$ within the Born approximation (first order perturbation theory in the scatterer strength). Specifically, we used $G_{k,k'} = G_0(k') (T(k) + T(k')) G_0(k)$. Here $G_0(k)$ is the Green’s function of a paired state in Nambu space and $T(k) = (\cos(k_x) - \cos(k_y)) \sigma_z$, where $\sigma_z$ is a Pauli matrix, models a local modulation of the pairing gap. (See ref. 30 for details of the calculations.) The phenomenological parameters used are: the band structure of ref. 57; a chemical potential leading to the Luttinger-count doping $p = 0.2$; a pairing gap $\Delta_0 = 20$ meV; a quasiparticle lifetime $\Gamma = 8$ meV. The sum over $k$ in equation (3) was performed by evaluating the summand over a grid of $200 \times 200$ points covering the square included between $(-5\pi, -5\pi)$ and $(5\pi, 5\pi)$. We verified that the numerical results are stable to small changes of the model, such as details of the phenomenological band structures, and small changes of the doping and of the pairing gap$^{30}$. In contrast, the specific choice of the impurity has important consequences for the shape of the $h$ maps (see Supplementary Section 7), highlighting the non-trivial relation between the source of disorder and the shape of the Friedel oscillations.

Data availability. The experimental data that support the plots within this paper and other findings of this study are available from the corresponding author upon request.

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