Echolocation by Quasiparticles

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It is shown that the local density of states (LDOS), measured in a Scanning Tunneling Microscopy (STM) experiment, at a single tip position contains oscillations as a function of energy, due to quasiparticle interference, which is related to the positions of nearby scatterers. We propose a method of STM data analysis based on this idea, which can be used to locate the scatterers. In the case of a superconductor, the method can potentially distinguish the nature of the scattering by a particular impurity.

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Scanning Tunneling Microscopy (STM), which measures the “local density of states” (LDOS) as a function of position and energy set by the bias voltage, has opened the door to imaging the sub-nanoscale topography and electronic structure of materials, including normal metals and especially cuprate superconductors. The technique is based on the fact that impurities produce spatial modulations of the LDOS in their vicinity — standing waves in the energy/time domain. Our analysis shows that the small particle oscillations were dominated by eight wavevectors that connect the tips of “banana” shaped energy contours in reciprocal space, the so-called Octet model as explained theoretically. For optimally doped samples, the dispersion inferred from these wavevectors agrees well with d-wave BCS theory indicating the existence of well-defined BCS quasiparticles in this regime.

The central observation of this paper is that the same Friedel-like oscillations of the LDOS, analyzed in the space/momentum domain by FT-STS, are also manifested in the energy/time domain. Our analysis shows that the small impurity-dependent modulations of the LDOS have a period, inversely proportional to the time required by a particle oscillations were dominated by eight wavevectors that connect the tips of “banana” shaped energy contours in reciprocal space, the so-called Octet model as explained theoretically. For optimally doped samples, the dispersion inferred from these wavevectors agrees well with d-wave BCS theory indicating the existence of well-defined BCS quasiparticles in this regime.

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The basic idea of the LDOS modulations may be understood semiclassically. The LDOS \( N(\mathbf{r}; \omega) \) is defined as \( -(1/\pi) \text{Im} G(\mathbf{r}, \mathbf{r}'; \omega) \), the time Fourier transform of the local (retarded) Green’s function \( G(\mathbf{r}, \mathbf{r}'; \omega) \). Imagine a bare electron wavepacket (centered on energy \( \omega \)) is injected at time \( t = 0 \) at point \( \mathbf{r} \) in a two-dimensional material: the Green’s function expresses its subsequent evolution. Assuming there are well-defined quasiparticles at this energy with dispersion \( E(\mathbf{k}) \); then for every wavevector \( \mathbf{k} \) on the energy contour \( E(\mathbf{k}) = \omega \), the wavepacket has a component spreading outwards at the group velocity \( v_g(\mathbf{k}) = \nabla_k E(\mathbf{k}) / \hbar \). When this ring reaches an impurity at \( \mathbf{r}_{\text{imp}} \), it serves as a secondary source and the reflected wavepacket arrives at the “echo time” \( T_e = 2 |\mathbf{R}| / |v_g(\mathbf{k})| \) for the \( \mathbf{k} \) such that \( v_g(\mathbf{k}) \parallel \mathbf{R} = \mathbf{r}_{\text{imp}} - \mathbf{r} \). This creates a sharp peak at \( t = T_e \) in \( G(\mathbf{r}, \mathbf{r}'; t) \) [see Fig. 1(d)], and hence modulations as a function of \( \omega \) in its Fourier transform \( \Delta N(\mathbf{r}; \omega) \) with period \( \Delta \omega = 2\pi \hbar / T_e \). Generally, for a particular impurity direction, \( |v_g| \) varies with energy, so the modulation in \( \Delta N(\omega) \) due to the impurity is “chirped” correspondingly.

We illustrate the quasiparticle echo first by a numerical calculation for a normal metal, defined by the lattice Schrodinger equation for the wavefunction \( u_i \) on site \( i \):

\[
\sum_j (t_{ij} + \mu_i \delta_{ij}) u_i = E u_i. \tag{2}
\]

Here the \( t_{ij}'s \) are intersite hoppings and the \( \mu_i's \) are on-site potentials (including the chemical potential); in this paper, we assume they are translationally invariant except at discrete (and dilute) impurity sites. We take the specific case of nearest-neighbor hopping \( t \) at half-filling, so the dispersion is \( E(k_x, k_y) = -2t(\cos k_x + \cos k_y) \), and we place one (repulsive site potential) impurity at the origin. To numerically calculate the LDOS, we used the Recursion method, which is well-suited for cases without translational symmetry.

Fig. 1(a) shows the impurity case LDOS which has echo oscillations on top of what otherwise would have been clean case LDOS, visible along the sides of the peak. Note that, for us to see more than one oscillation within the bandwidth, the impurity must be at least several sites away; hence the oscillations always have small amplitude and are best viewed by subtracting the clean LDOS. Throughout the paper, energy is in units of \( t \) and time in units of \( t^{-1} \) with \( t = 1 \) and \( \hbar = 1 \).

For a given energy \( \omega \), we define \( \Delta \omega(\omega)/2 \) as the separation of the zeros of that bracket \( \omega \) in the (subtracted) \( \delta N(\omega) \) trace, and let \( T_e(\omega) = 2\pi \hbar / \Delta \omega(\omega) \). We chose \( E = 0.7t \) and \( \mathbf{R} \) in the \([1,1]\) direction, for which the group velocity is \( v_g = 2.785t/\hbar \). Then, using \( \delta N(20, 20; \omega), \delta N(30, 30; \omega) \),
and $\delta N(40, 40; \omega)$ [the first and last trace of these are shown in Fig. 1(c,d)], we read off $\delta N(20, 20; \omega)$, $\delta N(40, 40; \omega)$, and $\delta N(\omega)$. The singularity appears at time $T_e/2$, where $T_e$ is given by (c). As we change the distance along this direction, the shortest echotime changes in proportion in accordance with our semiclassical expectations.

**Echolocation** — Using these quasiparticle echoes, we can locate the position of impurities by measuring the LDOS wiggles at a few points in the vicinity. At each point, we extract the wiggle period $\Delta \omega$ and hence the echo time $T_e \equiv 2\pi/\Delta \omega$. Then (1) defines a locus of possible impurity locations, $\{ \vec{r}_{\text{group}}(\vec{k})T_e/2 : \epsilon(\vec{k}) = \omega \}$. The intersection of the loci from STM spectra taken at multiple points $\vec{r}$ will locate $\vec{r}_{\text{imp}}$ uniquely. Furthermore, via a more exact derivation of the LDOS modulations (see below), the amplitude of the LDOS modulations tells the scattering strength of the impurities (in Born approximation they are proportional to each other). Once an impurity has been pin-pointed, the higher-energy STM spectrum at that point may independently identify the chemical nature of the impurity, e.g. in cuprates [15] and thus may reveal which kinds of impurities are important for the scattering of quasiparticles.

As a test, we evaluated the subtracted LDOS at three points $\vec{r}_A = (-30, 0)$, $\vec{r}_B = (-20, 20)$, and $\vec{r}_C = (15, 30)$, with the impurity at $\vec{r} = 0$. From the half-periods of the wiggles at energy $\omega = 0.7t$, (extracted as before) we found the respective echo times $T_A = 39.9$, $T_B = 20.4$ and $T_C = 36.7$. The three scaled loci (scaled by half the respective echotimes), shown in Fig. 2(e), intersect at $(0, 0)$ as can be seen graphically, thereby demonstrating the idea of echolocation. A more careful numerical analysis can be done to extract errors in echolocation as well.

**Analytic derivation** — Adopting the T-matrix formalism, we can obtain an analytic form for the LDOS modulations. Formally, the difference in dirty LDOS and clean LDOS for a single point impurity is given by

$$\delta N(\vec{r}; \omega) = -\frac{1}{\pi} \text{Im} \left[ G_0(\vec{r} - \vec{r}_{\text{imp}}; \omega)T(\omega)G_0(\vec{r}_{\text{imp}} - \vec{r}; \omega) \right]$$

where $G_0(\vec{r}, \vec{r}_{\text{imp}}; \omega) \equiv G_0(\vec{r} - \vec{r}_{\text{imp}}; \omega) \equiv G_0(\vec{R}; \omega)$ is the free propagator; LDOS modulations are due to interference between the two $G_0$ factors.

$$G_0(\vec{R}; \omega) = \lim_{\delta \to 0^+} \int_{B.Z.} \frac{dk_x dk_y}{(2\pi)^2} \frac{e^{i\vec{R} \cdot \vec{k}}}{\omega + i\delta - \epsilon(\vec{k})}$$

The integrand is singular all along the energy contour $\epsilon(\vec{k}) = \omega$, which we also parametrize as $k_y(s)$, where $s$ is the arc-length in reciprocal space. By the change of variables $z \equiv e^{ik_y}$ we convert the inner $(k_y)$ integral to a complex contour integral in the $z$ plane (rewriting $\epsilon(k_x, k_y)$ as an analytic function of $z$); for $k_x$ values found on the energy contour, the $z$ path encounters two poles, one inside and one outside, depending on the sign of $\delta$. Extracting the residue and absorbing factors, we get

$$G_0(\vec{R}; \omega) = \frac{1}{2\pi i} \int \eta(s)ds \frac{e^{i\vec{k}_s(s) \cdot \vec{R}}}{\hbar v_F(\vec{k}_s(s))} + G_{\text{non-singular}}$$

where $\eta(s) = 1$ on the half of the energy contour where $\text{sgn}(\delta) = \text{sgn}(|v_F(\omega, s)|)$ and zero on the other half. The non-singular term $G_{\text{non-singular}}$ comes from the integrals over $k_y$ which do not cross the energy contour.

At large $\vec{R}$, the two-dimensional BZ integration will be dominated by those $\vec{k}$ [18] on the energy contour where the
phase in the numerator is stationary, i.e. \( \mathbf{v}_g(\mathbf{k}) \parallel \mathbf{R} \); let us call such a point \( \mathbf{k}_R \) (so it is a function of the direction \( \mathbf{R} \) and of \( \omega \)). Using standard formulas of the stationary phase approximation [19] we get asymptotically

\[
G_0(\mathbf{R}; \omega) = \frac{-i e^{i \pi/4}}{v_g} \sqrt{\frac{1}{2\pi \kappa|\mathbf{R}|}} e^{i \mathbf{k}_R(\mathbf{R}; \omega) \cdot \mathbf{R}}. \tag{6}
\]

Here \( \kappa^{-1} \) is the curvature \( d^2 \mathbf{k}_R/d\mathbf{s}^2 \) of the energy contour at \( \mathbf{k}_R \).

Using (1) and (3), we finally get

\[
\delta N(\omega) = \frac{T}{2\pi^2 v_g^2 \kappa R} \cos \left( \frac{2 \mathbf{k}_R(\mathbf{R}, \omega) \cdot \mathbf{R}}{\mathbf{R}, \omega} \right). \tag{7}
\]

valid in the limit of a distant impurity. (All factors are actually functions of \( \mathbf{R} \) and \( \omega \); these arguments are shown only in the rapidly varying factors.) As we change \( \omega \) to \( \omega + \delta \omega \) keeping \( \mathbf{R} \) fixed, the chain rule gives \( \mathbf{k}_R(\omega + \delta \omega) - \mathbf{k}_R(\omega) = v_g^{-1} \delta \omega \mathbf{R} \) so, with \( \phi = \mathbf{k}_R \cdot \mathbf{R} \), we get

\[
\cos \left( \frac{2 \mathbf{k}_R(\mathbf{R}, \omega) \cdot \mathbf{R}}{\mathbf{R}, \omega} \right) \rightarrow \cos(\phi + T \delta \omega). \tag{8}
\]

This confirms the simple semiclassical prediction \( \Delta \omega = 2\pi/T_c \) (see Eq. (1)) for the modulation period due to echoes. The same quasiparticle interference is responsible for the spatial oscillations evident in (7) and the energy oscillations in (8).

**Echoes in cuprate superconductors** — Additional relevant issues arise in case of superconductors. To discuss these, we use a mean-field Bogoliubov-DeGennes(BDG) Hamiltonian with/without a single point impurity as shown below.

\[
\sum_j \begin{bmatrix} t_{ij} + \mu_i \delta_{ij} & \Delta_{ij}^* \\ \Delta_{ij} & -t_{ij} - \mu_i \delta_{ij} \end{bmatrix} \begin{bmatrix} u_i \\ v_i \end{bmatrix} = E \begin{bmatrix} u_i \\ v_i \end{bmatrix}, \tag{9}
\]

where we are using a lattice formulation of BDG equations. The \( u_i, s \) and \( v_i, s \) represent particle and hole amplitudes on site \( i \), \( t_{ij} \)s and \( \mu_i \)s represent the intersite hoppings and site chemical potentials respectively, and \( \Delta_{ij} \)s represent the off-diagonal order parameter amplitude. We discuss \( d \)-wave superconductors (dSCs) to highlight this method’s application to cuprates. For dSCs, \( \Delta_{ij} \) is nonzero only on nearest-neighbor bonds and \( \Delta_{i, \mathbf{k}, \pm} = -\Delta_{i, \mathbf{k}, \mp} \) because of the \( d \)-wave nature. Our normal state is the same nearest neighbor tight binding model on the square lattice with \( t = 1 \) and off-diagonal hopping amplitudes set to \( |\Delta| = 0.1 \). The Recursion method was extended to superconductors in [17] and is used for our numerics. In Fig. 3c and d), we show the LDOS(after subtracting the clean LDOS shown in Fig. 3a)) at \( 20 \sqrt{2} \) distance from an impurity along the \( (1, 1) \) direction for the case of a potential scatterer and an anomalous pair potential scatterer (which scatters an electron into a hole and vice versa) respectively.

In contrast to the normal case, there are two different wiggles: a fast one and a slow one. The reason for this is that the dSC quasiparticle dispersion gives rise to two different group velocities in the \( (1, 1) \) direction [20]. We also note that the fast wiggles exist only within the gap while the slow wiggles are both inside and outside the gap. In Fig. 3b), we show the constant energy contours for the quasiparticle dispersion given by \( E(\mathbf{k}) = \sqrt{\epsilon(\mathbf{k})^2 + |\Delta(\mathbf{k})|^2} \), the gradient of which is the quasiparticle group velocity. From Fig. 3b), we see that along \( (1, 1) \), the banana-shaped energy contours in the first and third quadrants give one velocity (which corresponds to the slow wiggles), while the contours in the second and fourth quadrants give a slower velocity (which corresponds to the fast wiggles). For \( E > |\Delta| \), there are no longer “banana” contours, so we get only one group velocity (similar to the normal case) and hence only one kind of wiggle is seen in Fig. 3c,d) outside the cusps.

Once the impurity is located using the loci intersection method described before, one can study the LDOS data around the impurity to infer the impurity’s strength and whether it is ordinary (magnetic/nonmagnetic) (cf. Ref. [21] and references therein) or anomalous [22]. This distinction is already visible in individual spectra: provided the normal state is particle-hole symmetric, one gets particle-hole symmetric echo oscillations \( \delta N_{ANO} \) from an anomalous impurity, since it scatters electrons into holes and vice versa [Fig. 3c,d)]; this is not the case for \( \delta N_{ORD} \) from an ordinary impurity [Fig. 3c,d].

A second diagnostic distinguishing (nonmagnetic) ordinary scatterers from anomalous ones is the real-space pattern of the surrounding standing waves in the LDOS, which is best seen in Born Approximation. In this limit, the impurity T-matrix is of the form (in the \( 2 \times 2 \) Nambu notation) \( U_{imp} T_{13} \) or \( T_{imp} T_{13} \) for the ordinary or anomalous cases, respectively. Then the echo oscillations take the respective forms

\[
\delta N_{ORD} \propto U_{imp}(G_{11}^2 - G_{12}^2); \quad \delta N_{ANO} \propto T_{imp}(2G_{11} G_{12}). \tag{10}
\]
Here, the $G_{ij}$s are the matrix elements of the usual free propagator $G_0(\vec{k}; \omega) = (\omega^2 - E(\vec{k})^2)^{-1} [\omega + \epsilon(\vec{k})\tau_3 + \Delta(\vec{k})\tau_1]$ thus in real space

$$G_0(\vec{R}; \omega) = \frac{\pi i}{(2\pi)^2} \int \frac{d^2 s}{2} g(\vec{R}(s, \omega)) + G_{\text{non-singular}}$$

We can carry out the stationary phase approximation as before, but instead we numerically calculated the propagator around an impurity over a grid of 20x20 lattice points (shown one quadrant with others related by symmetry).

We see that certain of the real-space oscillations, present in the case of the ordinary impurity, are suppressed in the case of a d-wave anomalous impurity. This is the same effect as the suppression of certain “octet” vectors [12, 13] for the case of d-wave anomalous impurity as argued in [22]’s Eq. 10 and the following paragraph. Our real-space analysis qualitatively duplicates that of Ref.22 illustrating how the real-space QPI and our energy-domain echoes are complementary manifestations of the same phenomenon.

**Conclusion and Discussion** — In conclusion, we have introduced a method of STM data analysis in the energy domain as a phenomenological tool for the study of real materials, complementary to FT-STS. Since it is based on the same quasiparticle interference effects already used successfully in FT-STS, we have confidence that the signals will be observable. They should be particularly strong in materials with an energy-dependent group velocity in some range of energies, such as d-wave superconductors and also graphene [23].

Since the echo analysis can be done in local patches of the sample (unlike FT-STS which fourier transforms over a larger region), we can locally verify the existence of quasiparticles at various energies through QPI. In particular, in cuprates, echoes might be used to check the hypothesis of quasiparticle extinction [24] above a certain energy. Furthermore, we have argued that echo analysis might reveal the nature of specific impurities [25] in a sample, information which hitherto was (at best) known statistically.

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