Quasiparticle scattering

Green’s function formalism

Garima Saraswat

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STM tip as a single atom electron source

$$H_0\phi = E\phi$$ Unperturbed Hamiltonian

Ref:Doyen G. (1996) The Scattering Theoretical Approach to the Scanning Tunneling Microscope

Fiete and Heller: Colloquium: Theory of quantum corrals and quantum mirages Rev. Mod. Phys., Vol. 75, 933, 2003

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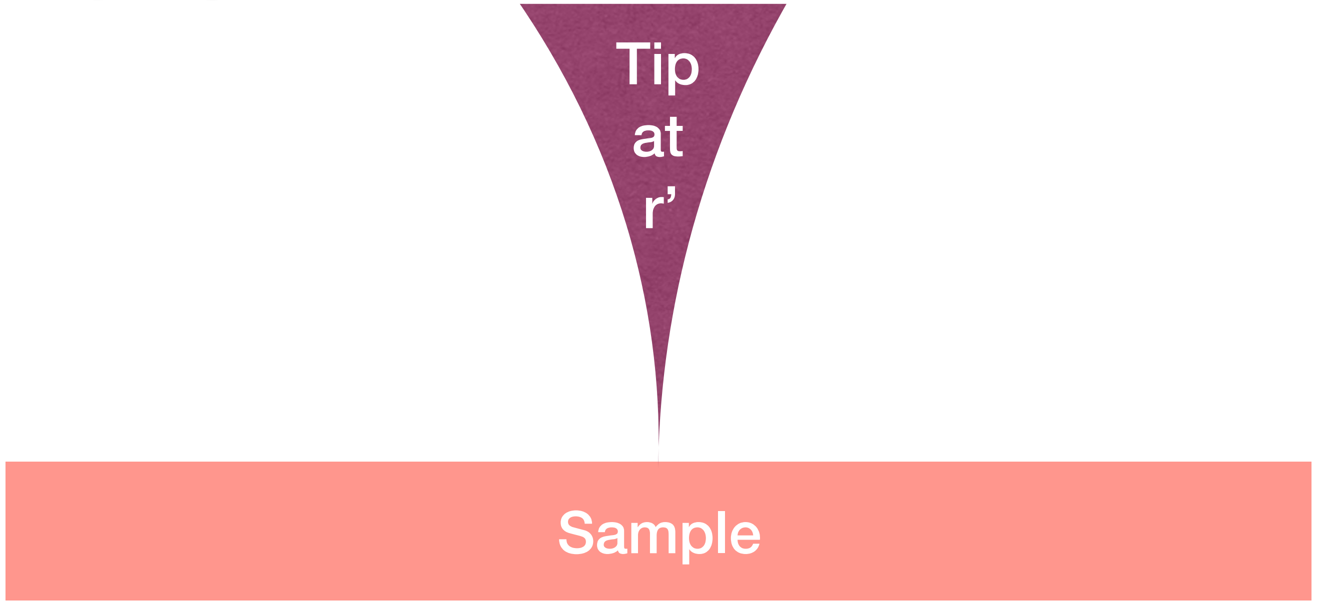
$$[E - H_0(r)]G_0(r, r', E) = \delta(r - r')$$ In presence of STM tip



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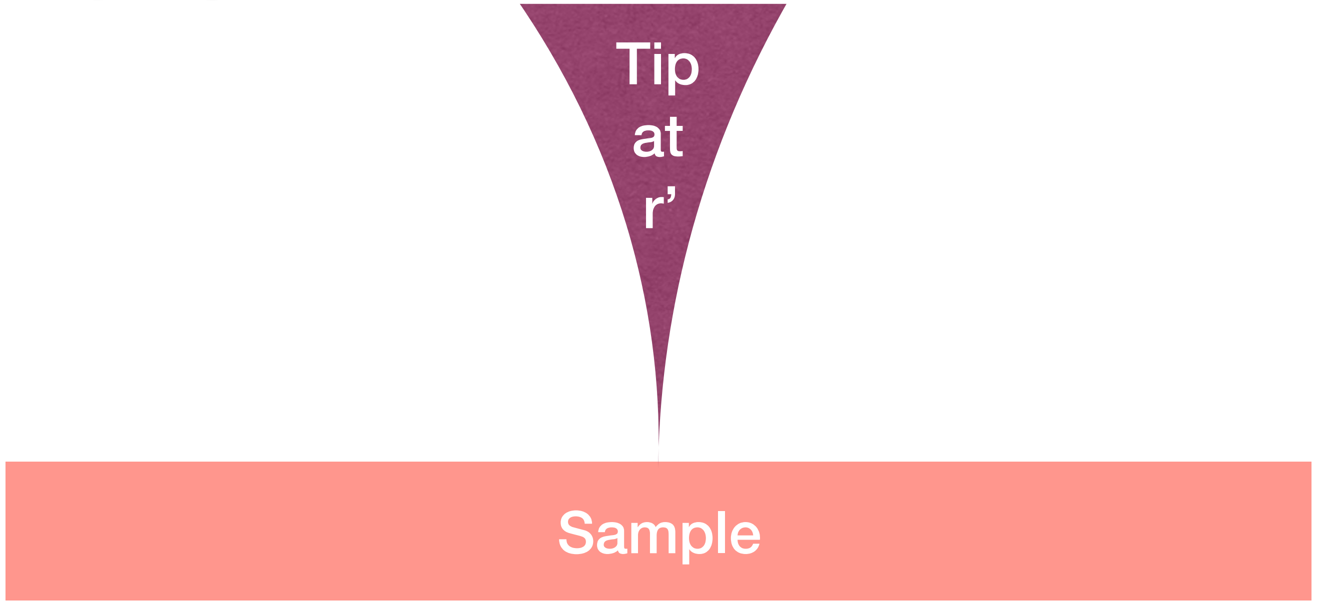
$$G_0(r, E) = \lim_{\epsilon \to 0^+} (E - H_0(r) + i\epsilon)^{-1}$$ satisfying causality



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G_0 for normal metal

2D : $H_0 = -\frac{\hbar^2}{2m^*}\left(\frac{d^2}{dx^2} + \frac{d^2}{dy^2}\right)$

$$G_0(r - r') = -i\frac{m^*}{2\hbar^2}[J_0(k\,|r - r'|) + iY_0(k\,|r - r'|)]$$

where $r = \sqrt{(x^2 + y^2)}$ and $k = \sqrt{2m^*(E - E_0)/\hbar^2}$

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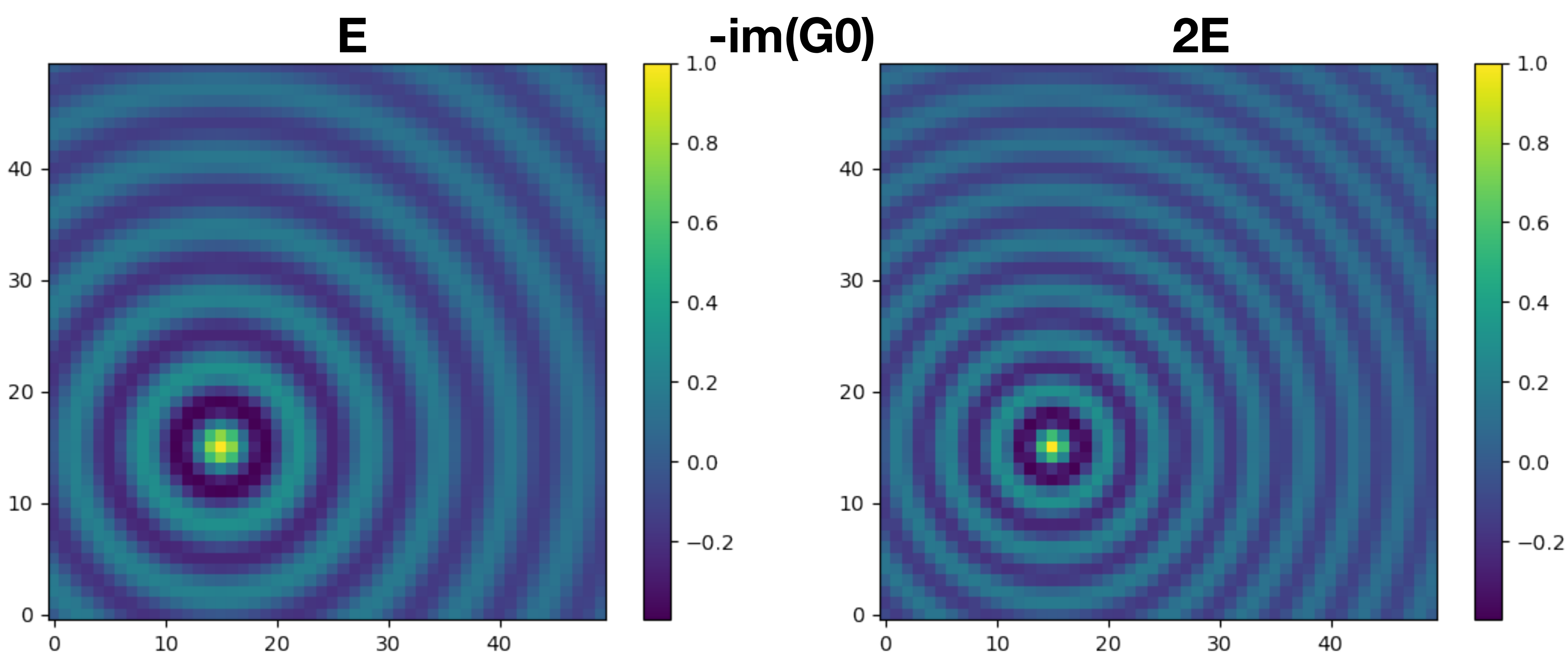

Tip position (15,15)

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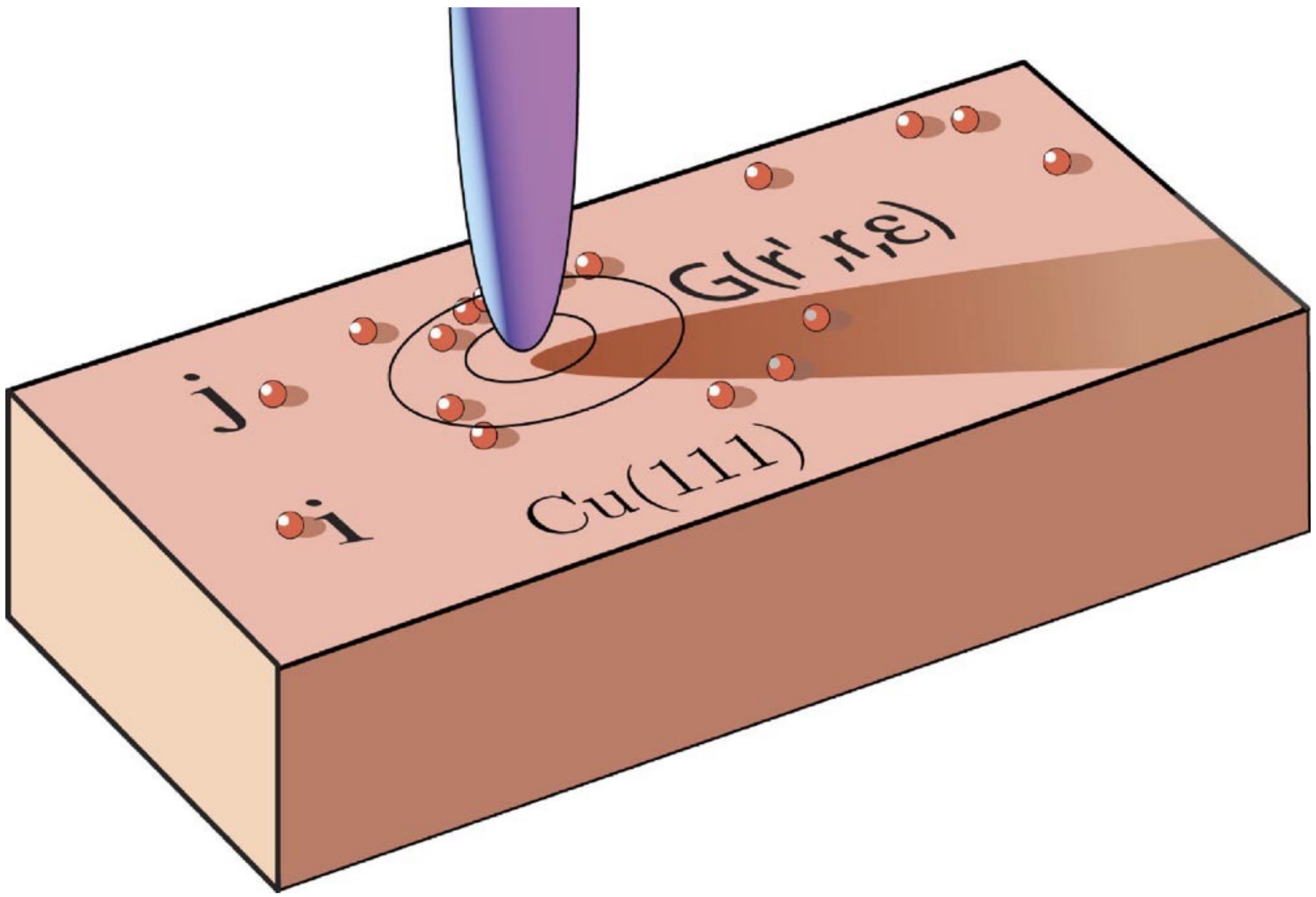
In presence of scatterer

$H = H_0 + V$ Hamiltonian with scattering potential

$G = G_0 + G_0 V G$ Dyson equation

$d(E) = -\lim_{\epsilon \to 0^+} \frac{1}{\pi} Im\, Tr(G)$ DOS

$\psi(x,y) = \phi(x,y) + \int\int dx' dy' G_0(x,y;x',y') V(x',y') \psi(x',y')$ Lippmann-Schwinger equation



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Numerical implementation

STS $\frac{\partial I}{\partial V} \propto \rho_{Tip} \int \left(\frac{\partial f(E-eV,T)}{\partial V} \right) \rho_{Sample}(E) dE$

LDOS $\rho(r) = \frac{-1}{\pi} ImG(r,r)$

$$G = (\mathbb{1} - G_0 V)^{-1} G_0$$

Numerical implementation

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In position basis:

$$\langle r|(E - H_0)G_0|r^{'}\rangle = \langle r|\mathbb{1}|r^{'}\rangle$$

$$\langle r|(E - H_0 + V)G|r^{'}\rangle = \langle r|\mathbb{1}|r^{'}\rangle$$

For 1D n sites: r varying from r_1 to r_n,
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For 2D lattice with n x n sites, r varies from r_1 to r_{n^2},
G_0, H_0, V, G are n^2 x n^2 matrices