Elastic Tunneling Theory

I present here a variation of the Bardeen and Tersoff-Hamann theories of elastic tunneling in STM. Suppose we have a system described by the Hamiltonian $H = H_0 + H'$. Then, by Fermi's Golden Rule, the rate of transitions from H_0 eigenstates $|i\rangle$ (the initial state with energy E_i) to $|f\rangle$ (a continuum of final states around energy E_f) is given by

$$dW = \sum_f \frac{2\pi}{\hbar} |\langle f|H'|i\rangle|^2 \delta(E_f - E_i) \tag{1}$$

Then, if we are tunneling from sample states $|s\rangle$ (with energies E_s) to STM tip states $|t\rangle$ (with energies E_t), the transition rate is

$$W = \sum_s \sum_t \frac{2\pi}{\hbar} |\langle t|H'|s\rangle|^2 \delta(E_t - E_s)(1 - f(E_t))f(E_s) \tag{2}$$

where $f(E)$ is the Fermi-Dirac Distribution.

Now, lets calculate the tunneling matrix element $\langle t|H'|s\rangle$. Define U_s to be the potential due to the sample and U_t to be due to the tip. Also assume that U_s and U_t do not overlap in space, i.e. $U_s = 0$ everywhere $U_t \neq 0$ and vice versa. Then, by simple application of the Schrödinger Equation,

$$\begin{aligned}
\langle t|H'|s\rangle &= \int_\tau \psi_t^* U_t \psi_s d^3\mathbf{r} = \int_\tau \left(\frac{\hbar^2}{2m} \nabla^2 \psi_t^* - E_t \psi_t^* \right) \psi_s d^3\mathbf{r} \\
&= \frac{\hbar^2}{2m} \int_\tau \left(\psi_t^* \nabla^2 \psi_s - \psi_s \nabla^2 \psi_t^* \right) d^3\mathbf{r} \\
&= \frac{\hbar^2}{2m} \int_\sigma \left(\psi_t^* \nabla \psi_s - \psi_s \nabla \psi_t^* \right) \cdot d\mathbf{A} \qquad (3)
\end{aligned}$$

where ψ_t and ψ_s represent tip and sample wavefunctions, respectively. The above integrals are taken over the entire volume τ such that $U_t \neq 0$, except for the last line, where the Divergence Theorem converts our volume integral into a flux integral over a surface σ between the tip and the sample. Note that I assumed $E_t = E_s$ because the $\delta(E_t - E_s)$ factor in the transition rate requires this to be so.
In the volume τ, $(\nabla^2 - \kappa^2)\psi_s = 0$, where $\kappa = (2m(\phi - E_s)/\hbar^2)^{1/2}$ and ϕ is the sample work function. If we assume the tip wavefunction obeys $(\nabla^2 - \kappa^2)\psi_t = -\delta(\mathbf{r} - \mathbf{r}_0)$, then

$$\psi_t(\mathbf{r}) = \frac{e^{-\kappa|\mathbf{r}-\mathbf{r}_0|}}{4\pi|\mathbf{r} - \mathbf{r}_0|} \tag{4}$$

In other words, we take the tip wavefunction to be an s-wave centered around the tip apex nucleus at $\mathbf{r}_0$. With this assumption, we find that $\langle t|H'|s\rangle \propto \psi_s(\mathbf{r}_0)$. Thus, the tunneling matrix element is proportional to the sample wavefunction evaluated at the tip apex.

Assuming the tip states form a continuum, we can replace the sum over t with an integral over dE_t,

$$W \propto \sum_s \int_{-\infty}^{\infty} |\psi_s(\mathbf{r}_0)|^2 D_t(E_t)\delta(E_t - E_s)(1 - f(E_t))f(E_s)dE_t \tag{5}$$

where $D_t(E_t)$ is the tip density of states.

If we apply a sample bias V, we must change this expression for W to reflect the fact that the sample electrochemical potential shifts by $-eV$. After doing the integral over dE_t,

$$W \propto \sum_s |\psi_s(\mathbf{r}_0)|^2 D_t(E_s)(1 - f(E_s))f(E_s + eV) \tag{6}$$

The total tunneling current $I(V)$ is $-e$ multiplied by the difference of the transition rate from sample to tip and from tip to sample. Thus,

$$I(V) \propto \sum_s |\psi_s(\mathbf{r}_0)|^2 D_t(E_s)(f(E_s) - f(E_s + eV)) \tag{7}$$

We assume the tip density of states is constant in the energy range of interest. We also assume low temperature so that $\frac{\partial}{\partial V} f(E_s + eV) \approx -e\delta(eV - (E_s - E_F))$, where E_F is the Fermi Energy. Then,

$$\frac{dI}{dV} \propto \sum_s |\psi_s(\mathbf{r}_0)|^2 \delta(eV - (E_s - E_F)) = \mathrm{LDOS}(\mathbf{r}_0, E_F + eV) \tag{8}$$

Therefore, $\frac{dI}{dV}$ can be interpreted as the local density of states.