The Local Density of States

There's this thing called the "Single Particle Green's Function" or "Feynman Propagator" or "Correlation Function". It is defined as

$$G(\mathbf{r}', t', \mathbf{r}, t) = -i\langle 0|T\{\Psi(\mathbf{r}, t)\Psi^\dagger(\mathbf{r}', t')\}|0\rangle \tag{1}$$

Here, $\mathbf{r}$ and $\mathbf{r}'$ are position vectors, $|0\rangle$ is the many body ground state with N electrons, and $\Psi^\dagger(\mathbf{r}', t')$ creates an electron while $\Psi(\mathbf{r}, t)$ destroys an electron. Ignore the T thing; it's called "time ordering" and is not relevant here. I will let $t' = 0$ and $t > 0$ just 'cause I can, and I will set $\hbar = 1$. In the Heisenberg picture, operators evolve as

$$\Psi(\mathbf{r}, t) = e^{iHt}\Psi(\mathbf{r})e^{-iHt} \tag{2}$$

$$\Psi^\dagger(\mathbf{r}, t) = e^{-iHt}\Psi^\dagger(\mathbf{r})e^{iHt} \tag{3}$$

so, putting this all together

$$G(\mathbf{r}', \mathbf{r}, t) = -i\langle 0|\Psi(\mathbf{r})e^{-iHt}\Psi^\dagger(\mathbf{r}')|0\rangle = -i\langle \mathbf{r}|e^{-iHt}|\mathbf{r}'\rangle \tag{4}$$

This has a physical interpretation. It is the probability amplitude that an electron starts at position $\mathbf{r}'$, then is subject to time evolution for time t, and ends up at position $\mathbf{r}$. Now, lets suppose we have a complete set of $N + 1$ electron energy eigenstates denoted by $\{|\lambda\rangle\}$. They have energies $\{E_\lambda\}$. The resolution of the identity says $1 = \sum_\lambda |\lambda\rangle\langle\lambda|$.

$$G(\mathbf{r}', \mathbf{r}, t) = -i\sum_{\lambda\lambda'}\langle \mathbf{r}|\lambda\rangle\langle\lambda|e^{-iHt}|\lambda'\rangle\langle\lambda'|\mathbf{r}'\rangle = -i\sum_\lambda e^{-iE_\lambda t}\psi^*_\lambda(\mathbf{r}')\psi_\lambda(\mathbf{r}) \tag{5}$$

Now let $\mathbf{r}' = \mathbf{r}$ because STM injects/removes electrons at the same position that it makes its measurement. Also, an STM measurement is "slow" in that a measurement timescale is much longer than the time it takes for dynamics on the surface to happen. Thus, we should Fourier Transform the Green's Function.

$$G(\mathbf{r}, \omega) = -i\sum_\lambda\int_0^\infty e^{i(\omega - E_\lambda)t}e^{-\delta t}|\psi_\lambda(\mathbf{r})|^2 dt \tag{6}$$

Note that I put in $e^{-\delta t}$ to help the integral converge. Physically, $1/\delta$ is the lifetime of a quasiparticle excitation. We will take the limit wherer δ goes to zero at the end of the calculation.

$$G(\mathbf{r}, \omega) = -i\sum_\lambda\left[\frac{e^{i(\omega - E_\lambda)t}e^{-\delta t}}{i(\omega - E_\lambda) - \delta}\right]_0^\infty |\psi_\lambda(\mathbf{r})|^2 = -\sum_\lambda\left[\frac{1}{\omega - E_\lambda + i\delta}\right]|\psi_\lambda(\mathbf{r})|^2 \tag{7}$$

Define the "Spectral Function"

$$A(\mathbf{r}, \omega) = \frac{1}{\pi}\mathrm{Im}[G(\mathbf{r}, \omega)] = \frac{1}{\pi}\sum_\lambda\frac{\delta}{(\omega - E_\lambda)^2 + \delta^2}|\psi_\lambda(\mathbf{r})|^2 \tag{8}$$

You might notice the similarity to the ARPES spectra function

$$A(k, \omega) = \frac{1}{\pi}\mathrm{Im}[G(k, \omega)] = \frac{1}{\pi}\frac{\mathrm{Im}\Sigma}{(\omega - E_k - \mathrm{Re}\Sigma)^2 + (\mathrm{Im}\Sigma)^2} \tag{9}$$

Anyway, take the $\delta \to 0$ limit, and $\frac{1}{\pi} \sum_{\lambda} \frac{\delta}{(\omega - E_\lambda)^2 + \delta^2} \to \delta(\omega - E_\lambda)$, where $\delta(\omega - E_\lambda)$ is the Dirac Delta Function. Finally, we get the Local Density of States

$$A(\mathbf{r}, \omega) = \sum_{\lambda} |\psi_\lambda(\mathbf{r})|^2 \delta(\omega - E_\lambda) = \mathrm{LDOS}(\mathbf{r}, \omega) \tag{10}$$

I probably lost some proportionality factors, but they don't matter because dI/dV is only proportional to LDOS anyway.