Magnesium diboride (MgB_2)

- Conventional superconductor with special features
  - double gap model
  - highest Tc among BCS superconductors (39K)

MgB_2 thin films

- Two samples (#2, #3) out of three have undergone neutron scattering:
  - destroys anisotropy
  - makes film properties similar to a single-gap BCS superconductor

BCS model predictions

- Single gap, plus a phenomenological parameter (Dynes' Γ)

BCS model predictions

$$\nu_{(\Gamma,\Delta)}(E) \equiv \frac{N(E)}{N(0)} = \left|\Re\left(\frac{E - i\Gamma}{\sqrt{(E-i\Gamma)^2 - \Delta^2}}\right)\right|$$

$$f(u) = \frac{1}{\exp(u)+1}, \text{ con } u = \frac{E}{k_B T}$$

$$\left(\frac{dI}{dV}\right)_{(\Gamma,\Delta)}(V) = \frac{1}{k_B T}\int \nu_{(\Gamma,\Delta)}(E)\left(-\frac{df}{du}\left(\frac{E-eV}{k_B T}\right)\right) dE$$

Double gap

- DoS (hence, dI/dV) as a linear combination of two single-gap Densities of States
  - "normalized" coefficients $\alpha_\pi + \alpha_\sigma = 1$
  - w/ constraint $0.66 < \alpha_\pi < 1$

$$\left(\frac{dI}{dV}\right)^{MgB_2}_{(\Gamma_\pi,\Delta_\pi,\Gamma_\sigma,\Delta_\sigma,\alpha_{\pi|\sigma})}(V) =$$

$$\alpha_\pi \left(\frac{dI}{dV}\right)_{(\Gamma_\pi,\Delta_\pi)}(V) + \alpha_\sigma \left(\frac{dI}{dV}\right)_{(\Gamma_\sigma,\Delta_\sigma)}(V)$$

Computational difficulties

- The conductivity curve depends non linearly on Γ and Δ through a *numerical* integral (no analytical solution)
- Double-gap model leads to five independent parameters: Γ_π, Δ_π, Γ_σ, Δ_σ, and one coefficient e.g. α_π

Finding the best fit (method 1)

- Simplex
  - most powerful method, with limitations
  - doesn't need derivatives
  - χ^2 is “yet another function” to find a minimum for
  - *can't* estimate statistical errors

Finding the best fit (method 2)

- `gsl_multifit_*()`
  - not a generic minimization procedure
  - less robust than *Simplex* on "irregular" functions but...
  - ...<u>can estimate statistical covariances and sigmas!</u>
  - min $\chi^2(\Gamma_\pi, \Delta_\pi, \Gamma_\sigma, \Delta_\sigma, \alpha_\pi)$ ***Levenberg-Marquardt***

Best of both worlds?

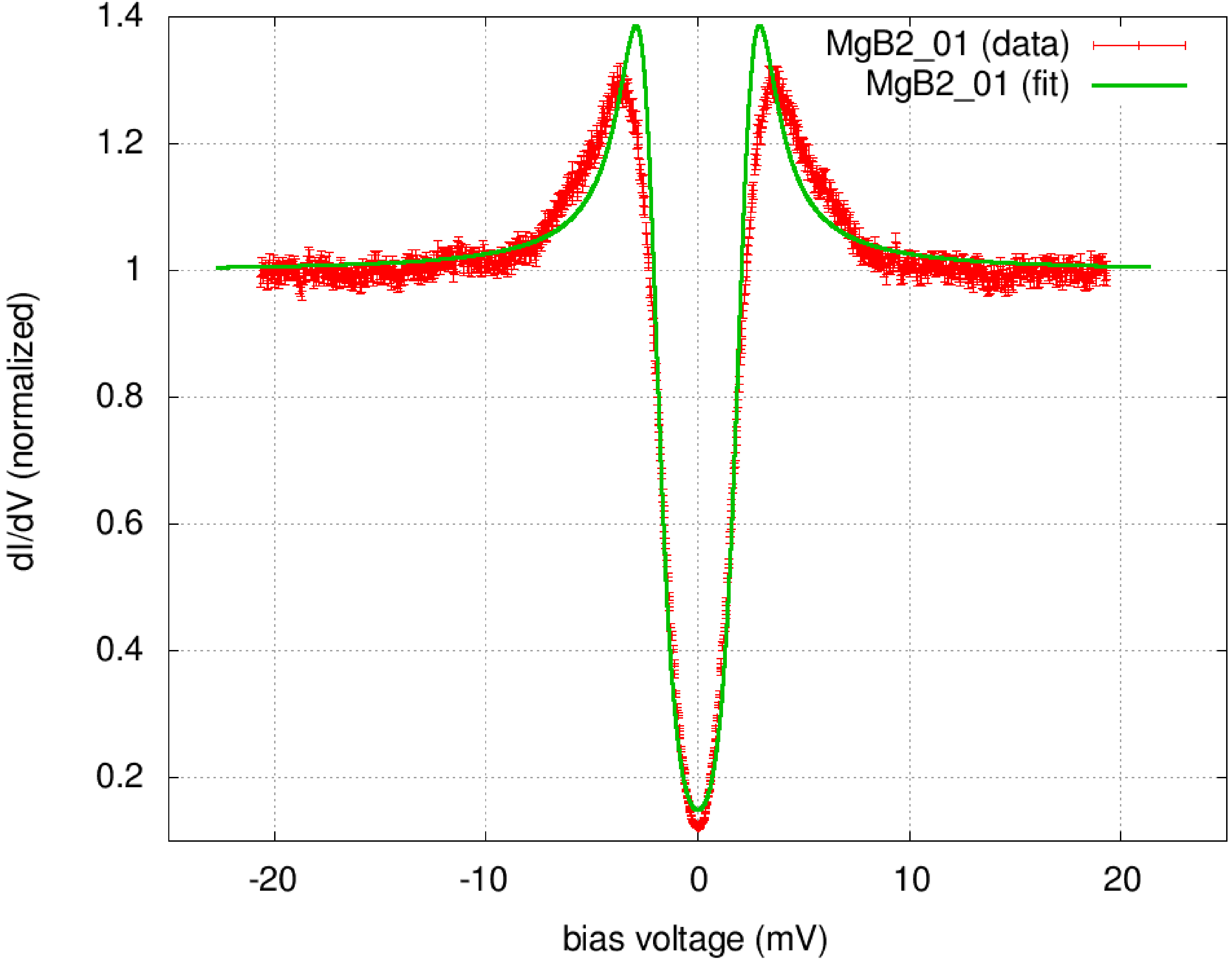
- Simplex method to find a good minimum
- Starting from the last result, `gsl_multifit_fdfsolver_iterate()` to (slightly) improve the fit, but most importantly compute statistical errors

https://www.youtube.com/watch?v=LLLq7-0DivI

https://bitbucket.org/gderosa/didvsuperc/src

Results

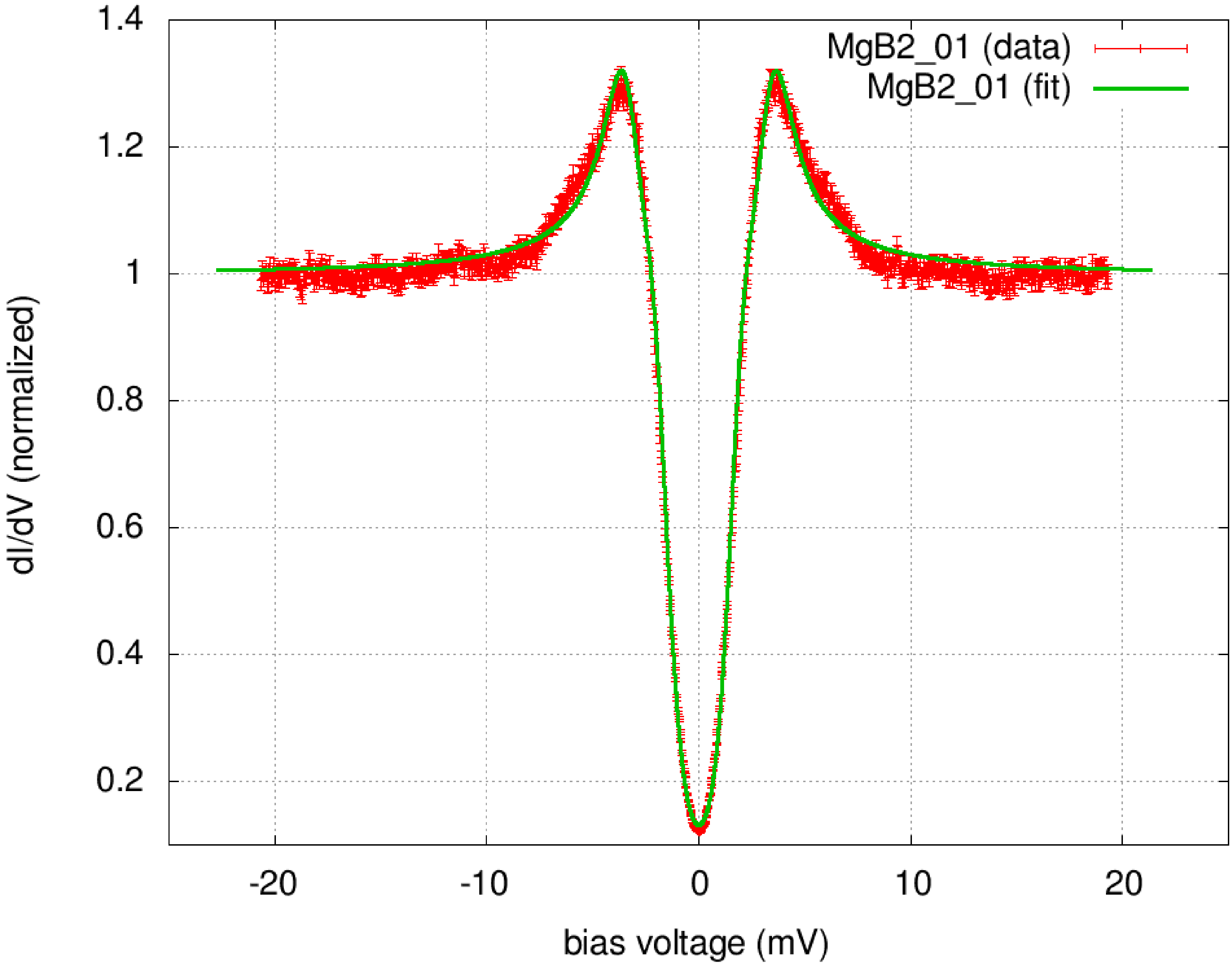
- Sample #1; single gap
  - $\Gamma = 0.2639 \pm 0.0023$
  - $\Delta = 2.2327 \pm 0.0023$
  - $\chi^2/DoF = 17.669$



MgB2_01 (data)
MgB2_01 (fit)
dI/dV (normalized)
bias voltage (mV)
1.4
1.2
1
0.8
0.6
0.4
0.2
-20
-10
0
10
20

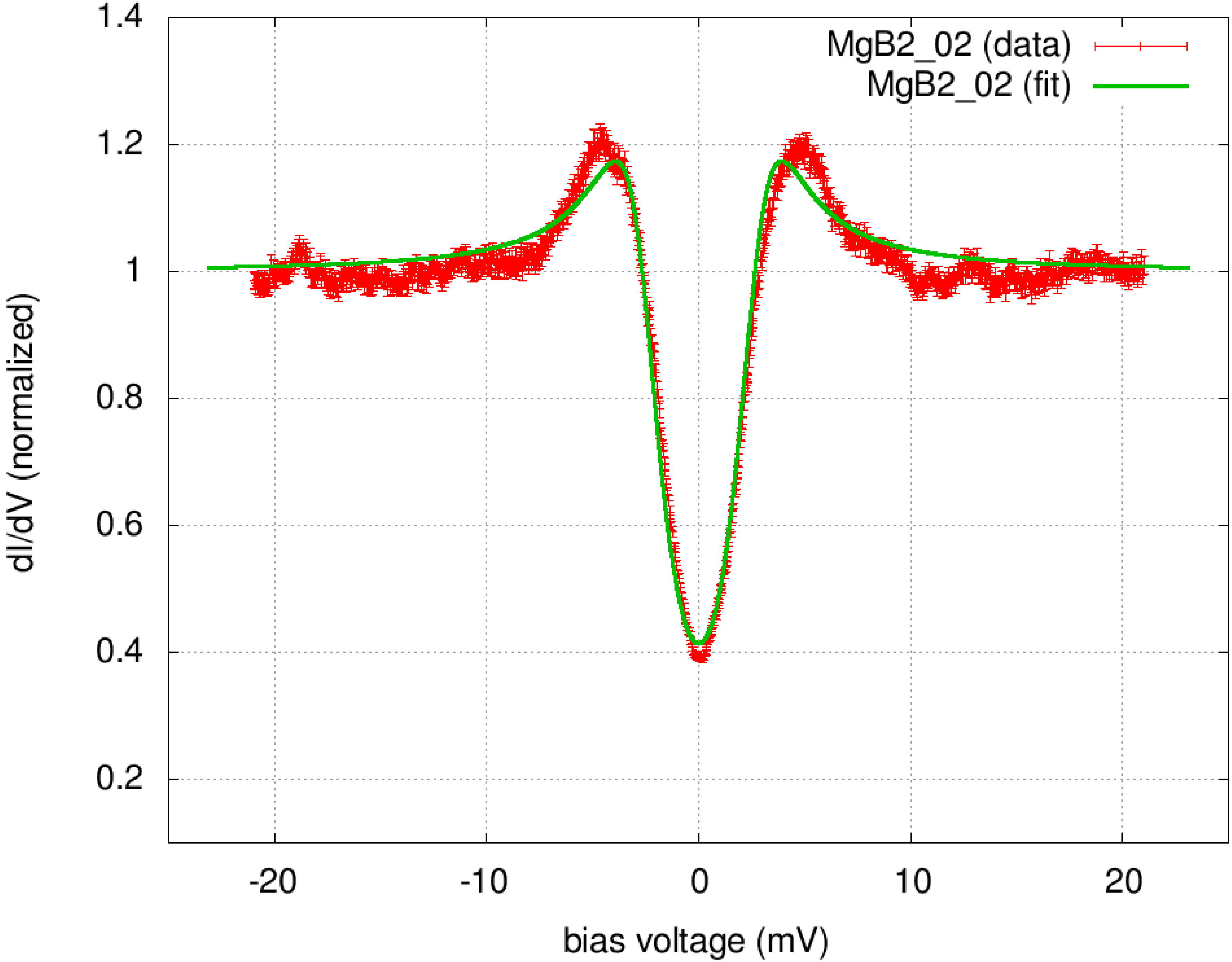
A better fit with a double gap

- Sample #1; <u>double gap</u>
  - Γ = 0.1866±0.0019
  - Δ_π = 1.7895±0.0050
  - Δ_σ = 3.2348±0.0073
  - α_π = 0.6660±0.0027
  - χ^2/DoF= 3.4737

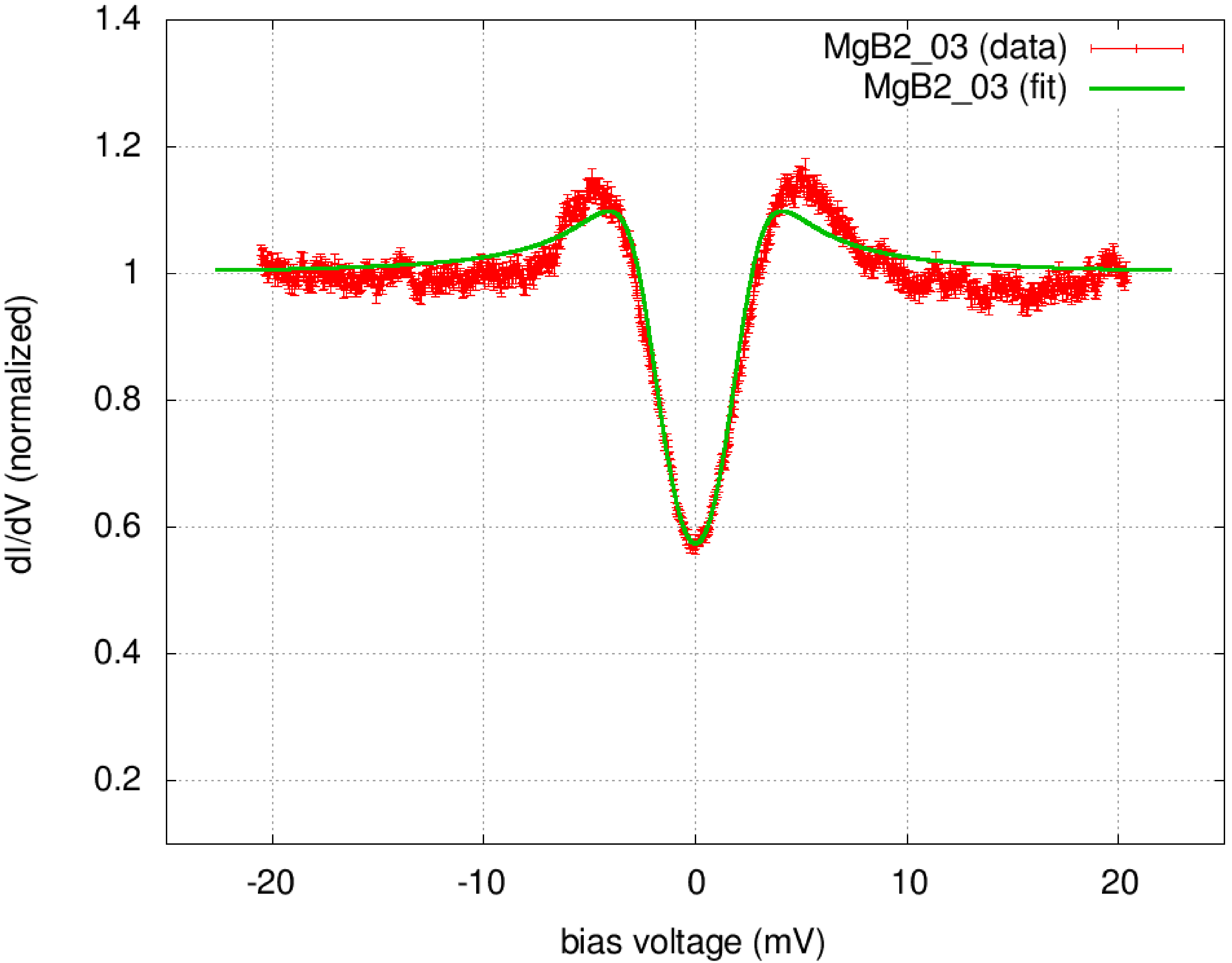

MgB2_01 (data)
MgB2_01 (fit)
dI/dV (normalized)
bias voltage (mV)
1.4
1.2
1
0.8
0.6
0.4
0.2
-20
-10
0
10
20

The single gap model fits better with “disordered” (neutron-scattered) films

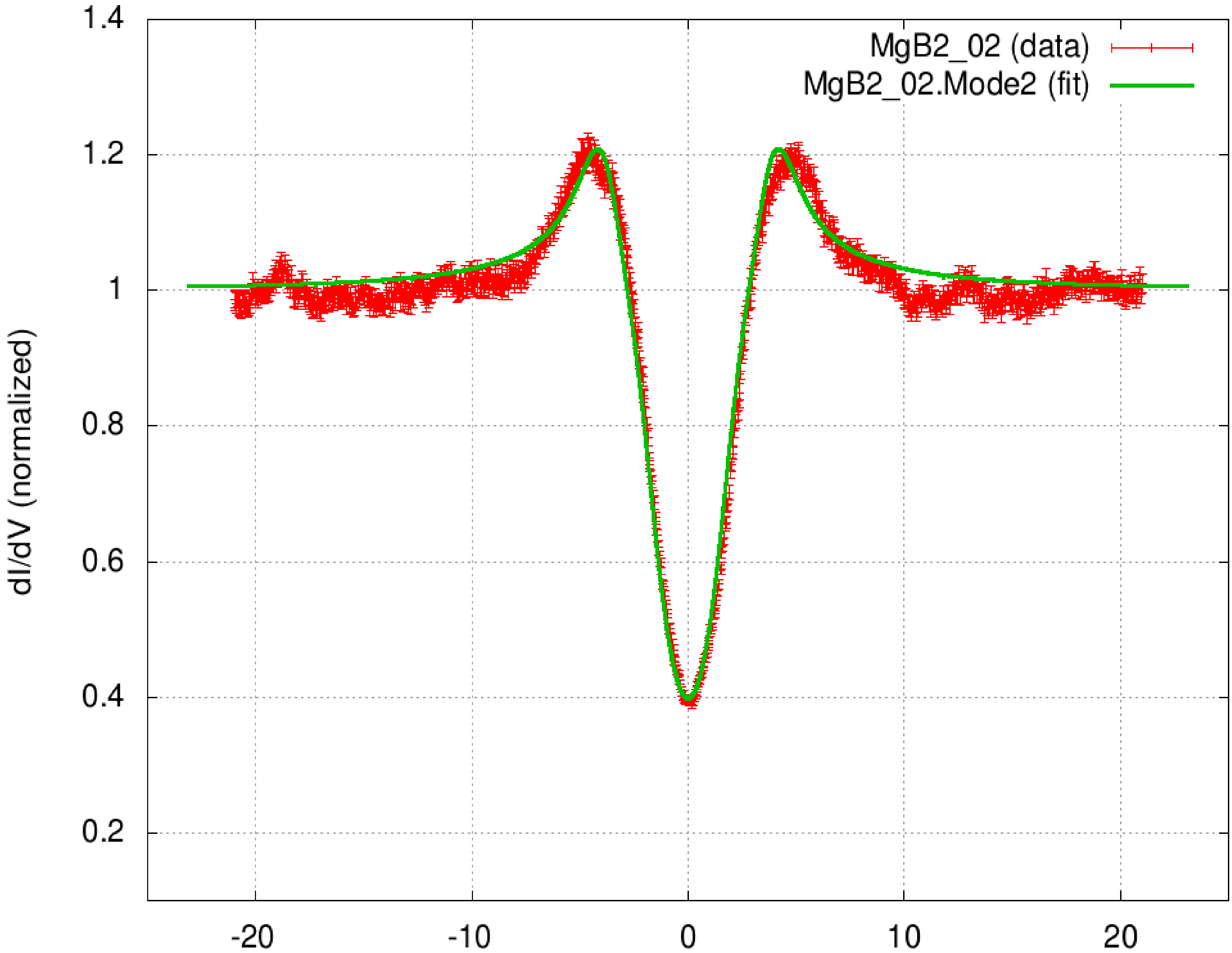
Samples #2 and #3, single-gap first (Γ, Δ), then double-gap (Γ_π, Δ_π, Γ_σ, Δ_σ, α_π)



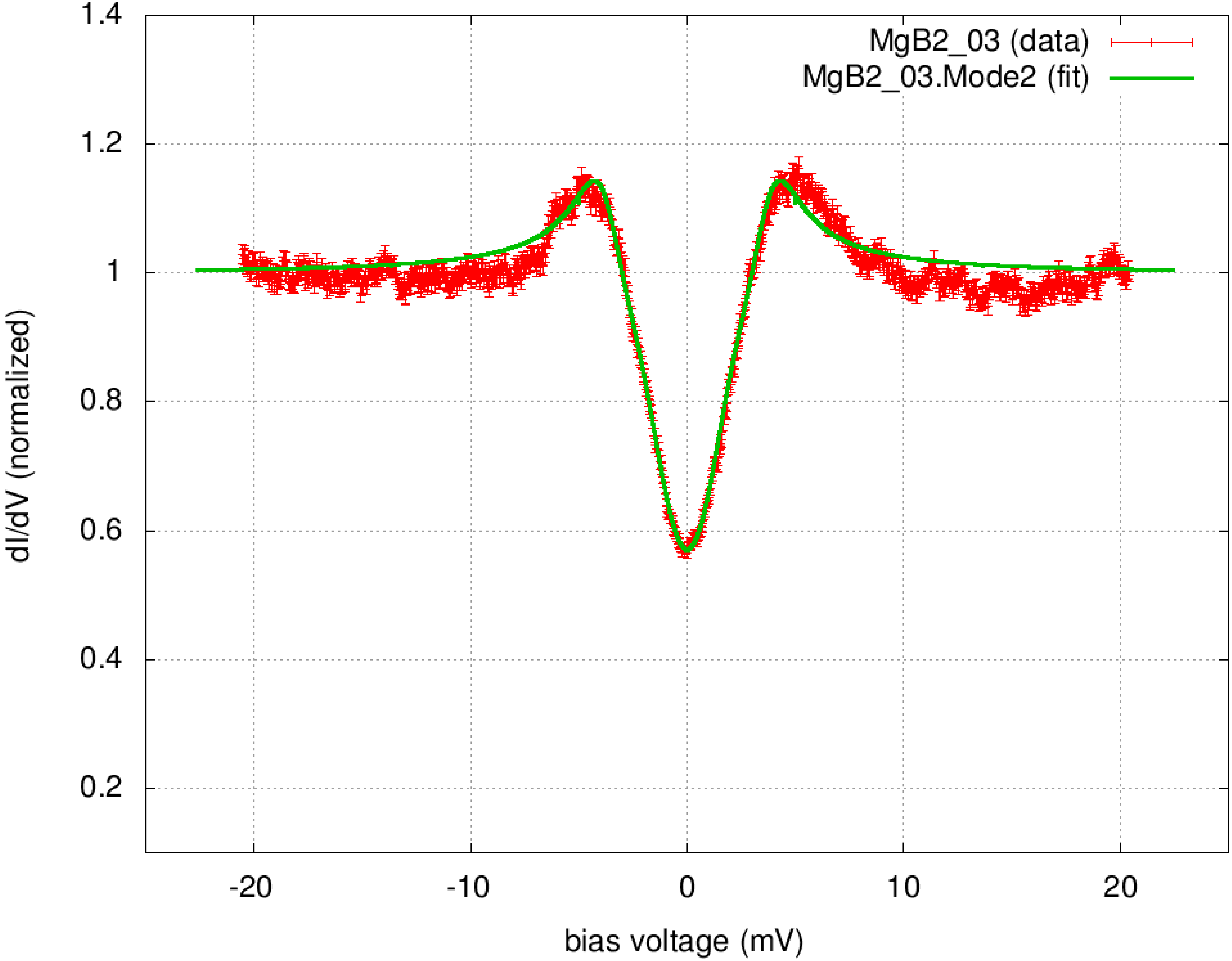
MgB2_02 (data)
MgB2_02 (fit)
dI/dV (normalized)
bias voltage (mV)
1.4
1.2
1
0.8
0.6
0.4
0.2
-20
-10
0
10
20



MgB2_03 (data)
MgB2_03 (fit)
dI/dV (normalized)
bias voltage (mV)
1.4
1.2
1
0.8
0.6
0.4
0.2
-20
-10
0
10
20



MgB2_02 (data)
MgB2_02.Mode2 (fit)
dI/dV (normalized)
1.4
1.2
1
0.8
0.6
0.4
0.2
-20
-10
0
10
20



MgB2_03 (data)
MgB2_03.Mode2 (fit)
dI/dV (normalized)
bias voltage (mV)
1.4
1.2
1
0.8
0.6
0.4
0.2
-20
-10
0
10
20

Results

	MgB2_01	MgB2_02	MgB2_03
Γ	0.2639 ± 0.0023	1.0753 ± 0.0037	1.4726 ± 0.0054
Δ	2.2327 ± 0.0023	2.5983 ± 0.0035	2.2969 ± 0.0053
$\tilde{\chi}^2$	17.669	5.0787	4.8334
Γ	0.1866 ± 0.0019	0.901 ± 0.013	0.590 ± 0.017
Δ_π	1.7895 ± 0.0050	2.018 ± 0.022	0.8620 ± 0.0094
Δ_σ	3.2348 ± 0.0073	3.433 ± 0.032	3.406 ± 0.019
α_π	0.6660 ± 0.0027	0.6661 ± 0.0064	0.6687 ± 0.0054
$\tilde{\chi}^2$	3.4737	4.4335	4.3942
Γ_π	0.2013 ± 0.0055	0.946 ± 0.012	1.297 ± 0.021
Γ_σ	0.086 ± 0.028	0.350 ± 0.075	0.452 ± 0.081
Δ_π	1.7591 ± 0.0063	2.025 ± 0.024	1.643 ± 0.031
Δ_σ	3.178 ± 0.011	3.664 ± 0.039	3.650 ± 0.042
α_π	0.666 ± 0.011	0.794 ± 0.019	0.813 ± 0.017
$\tilde{\chi}^2$	3.2813	4.1305	3.5091