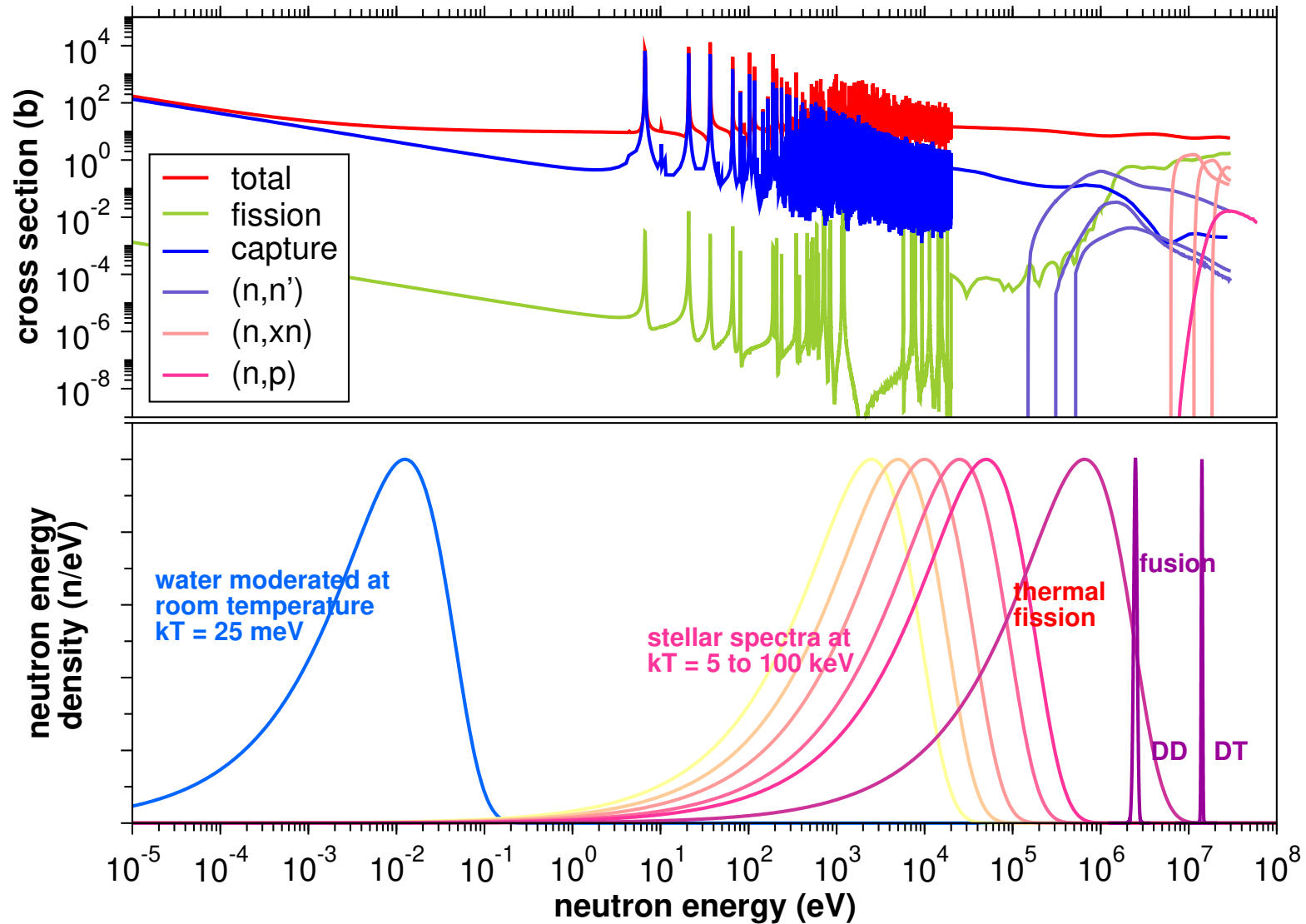


Considerations on resolved neutron resonance fitting

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The Breit-Wigner Single Level approximation:

total cross section:

$$\sigma_c = \pi \lambda_c^2 g_c \left(4 \sin^2 \phi_c + \frac{\Gamma_\lambda \Gamma_{\lambda c} \cos 2\phi_c + 2(E - E_\lambda - \Delta_\lambda) \Gamma_{\lambda c} \sin 2\phi_c}{(E - E_\lambda - \Delta_\lambda)^2 + \Gamma_\lambda^2 / 4} \right)$$

- neutron channel: $c = n$
- if only capture, scattering, fission: $\Gamma_\lambda = \Gamma = \Gamma_n + \Gamma_\gamma + \Gamma_f$
- other approximations:

$$\ell = 0 \quad \cos \phi_c = 1 \quad \sin \phi_c = \rho = ka_c \quad \Delta_\lambda = 0$$

total cross section for s-wave at temperature 0 K:

$$\sigma_T(E) = \overbrace{4\pi R'^2}^{\text{potential}} + \pi \lambda^2 g \left(\frac{\overbrace{4\Gamma_n(E - E_0)R'/\lambda}^{\text{interference}} + \overbrace{\Gamma_n^2}^{\text{elastic}} + \overbrace{\Gamma_n\Gamma_\gamma}^{\text{capture}} + \overbrace{\Gamma_n\Gamma_f}^{\text{fission}}}{\underbrace{(E - E_0)^2 + (\Gamma_n + \Gamma_\gamma + \Gamma_f)^2 / 4}_{\text{total width}}} \right)$$

Parametrization of single isolated resonance

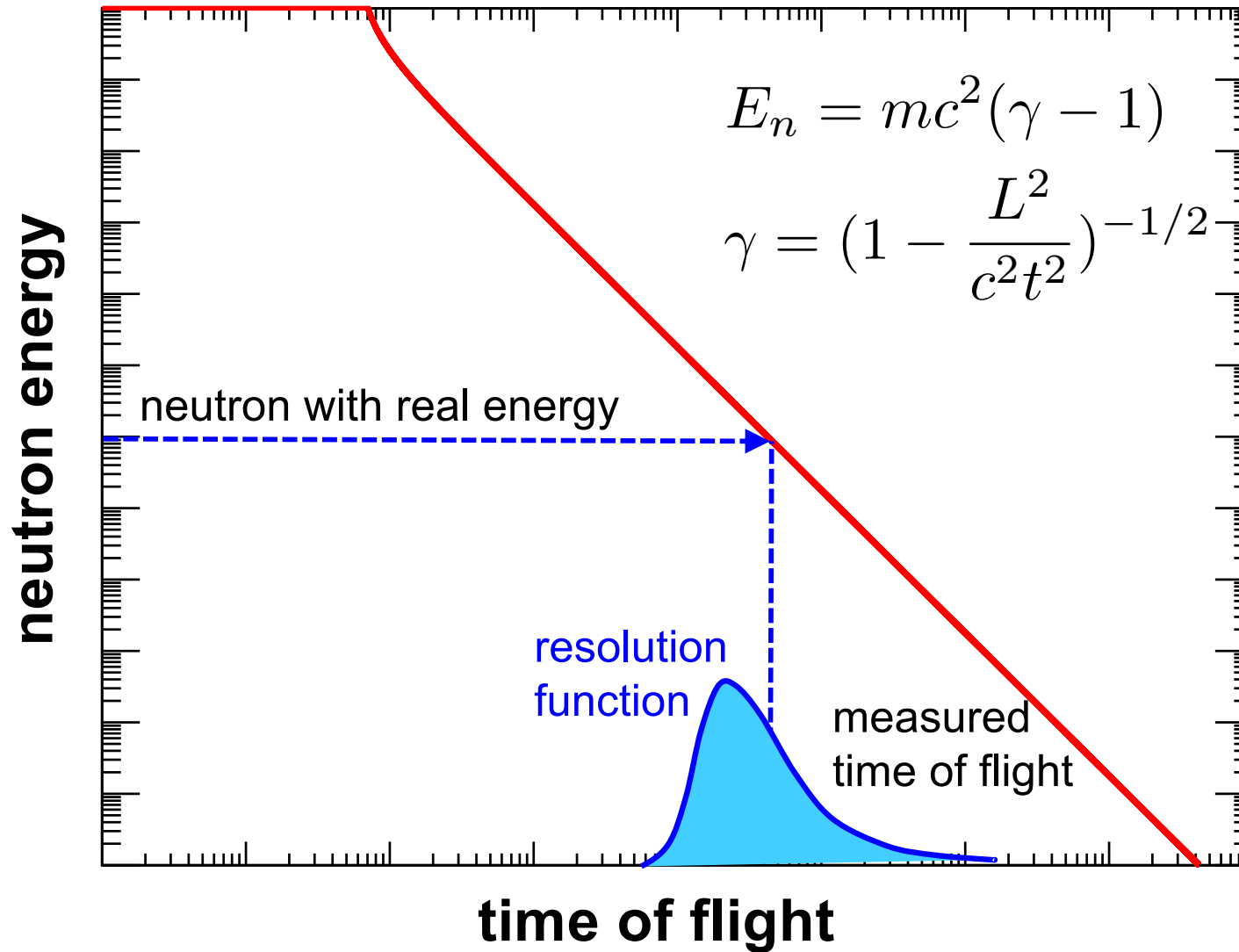
- cross sections at **0 K** are a function of resonance parameters:

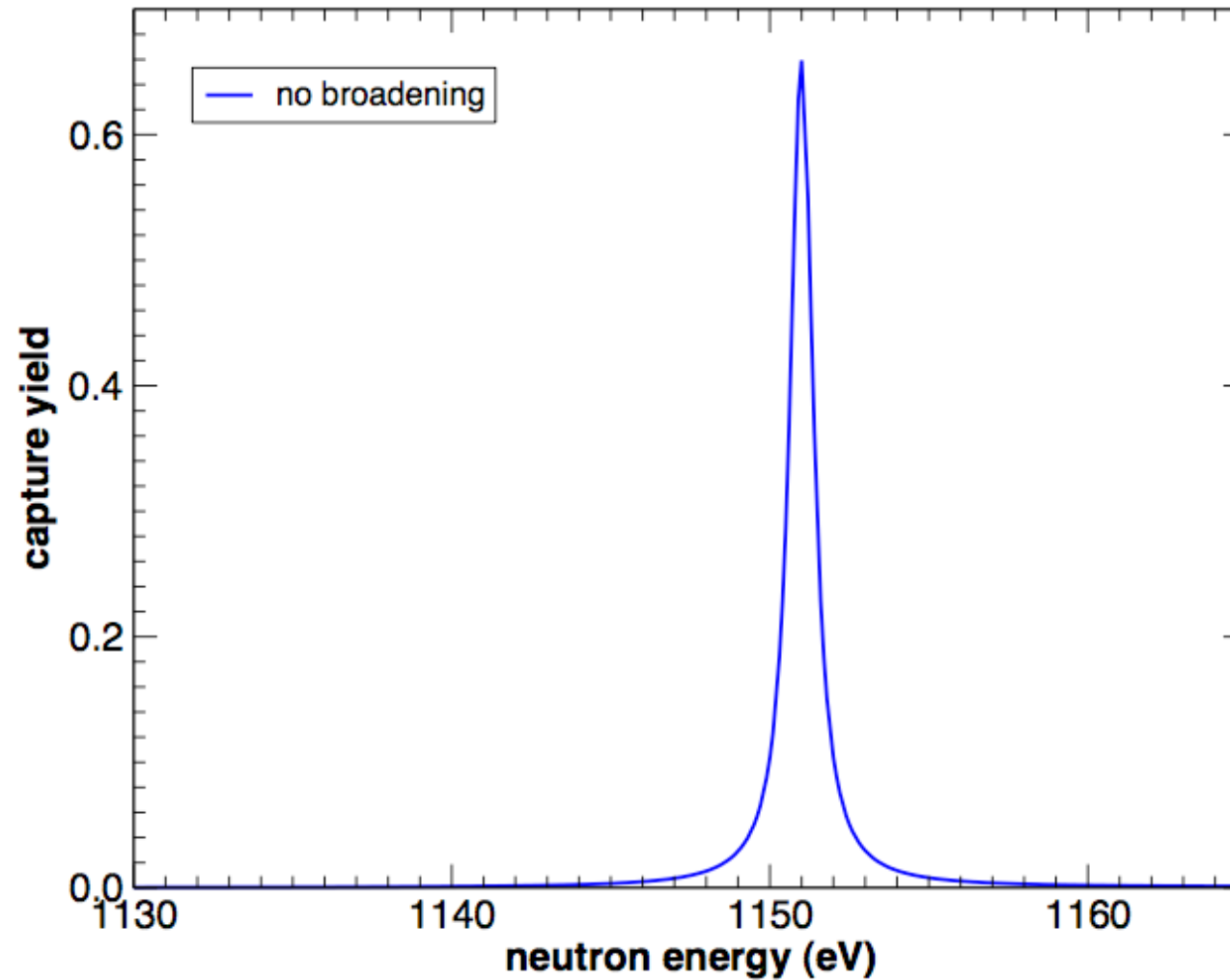
- partial and/or total widths $\Gamma_n, \Gamma_\gamma, \Gamma_f, \Gamma$

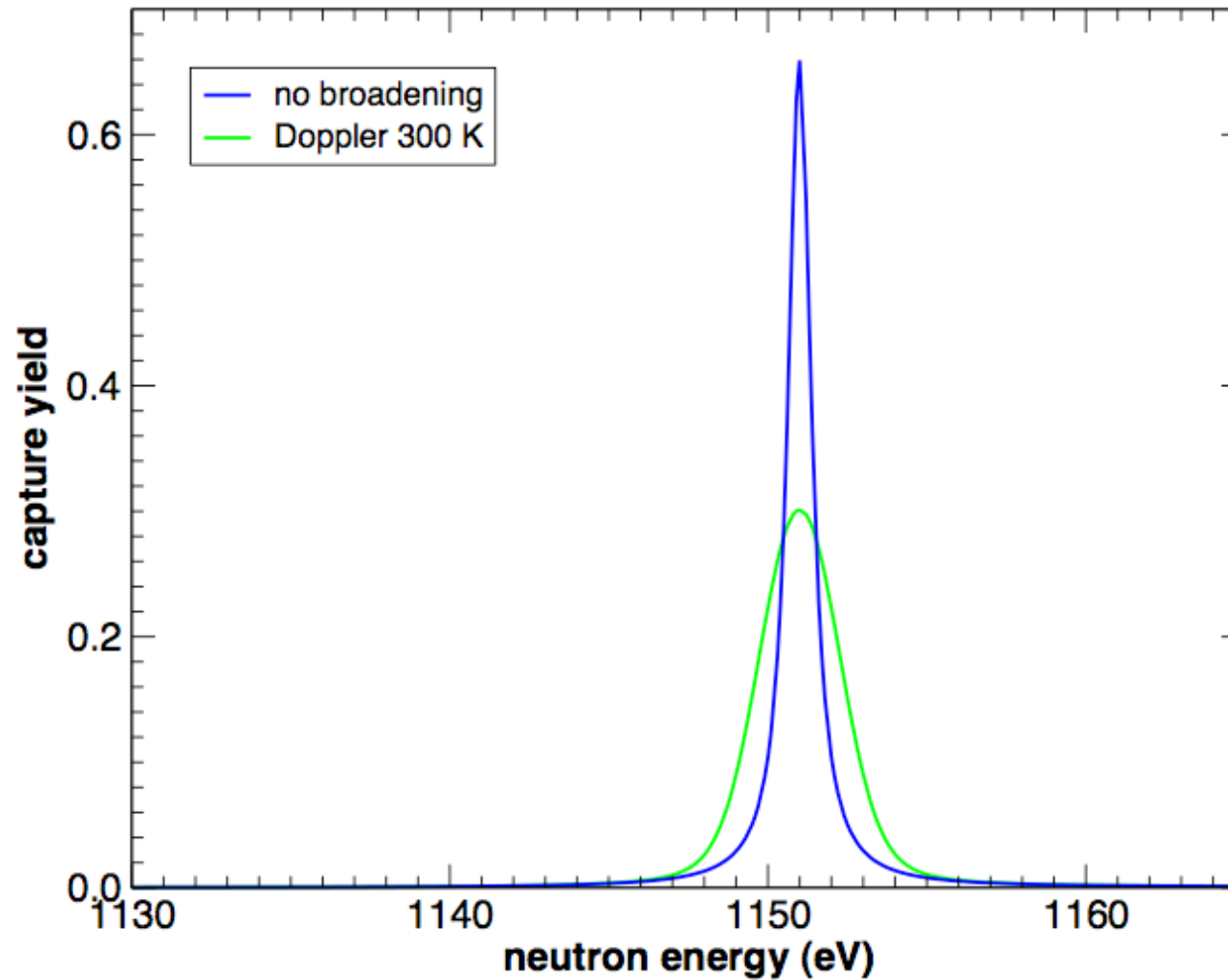
- spin, (channel spin), parity, orbital momentum or derived quantities

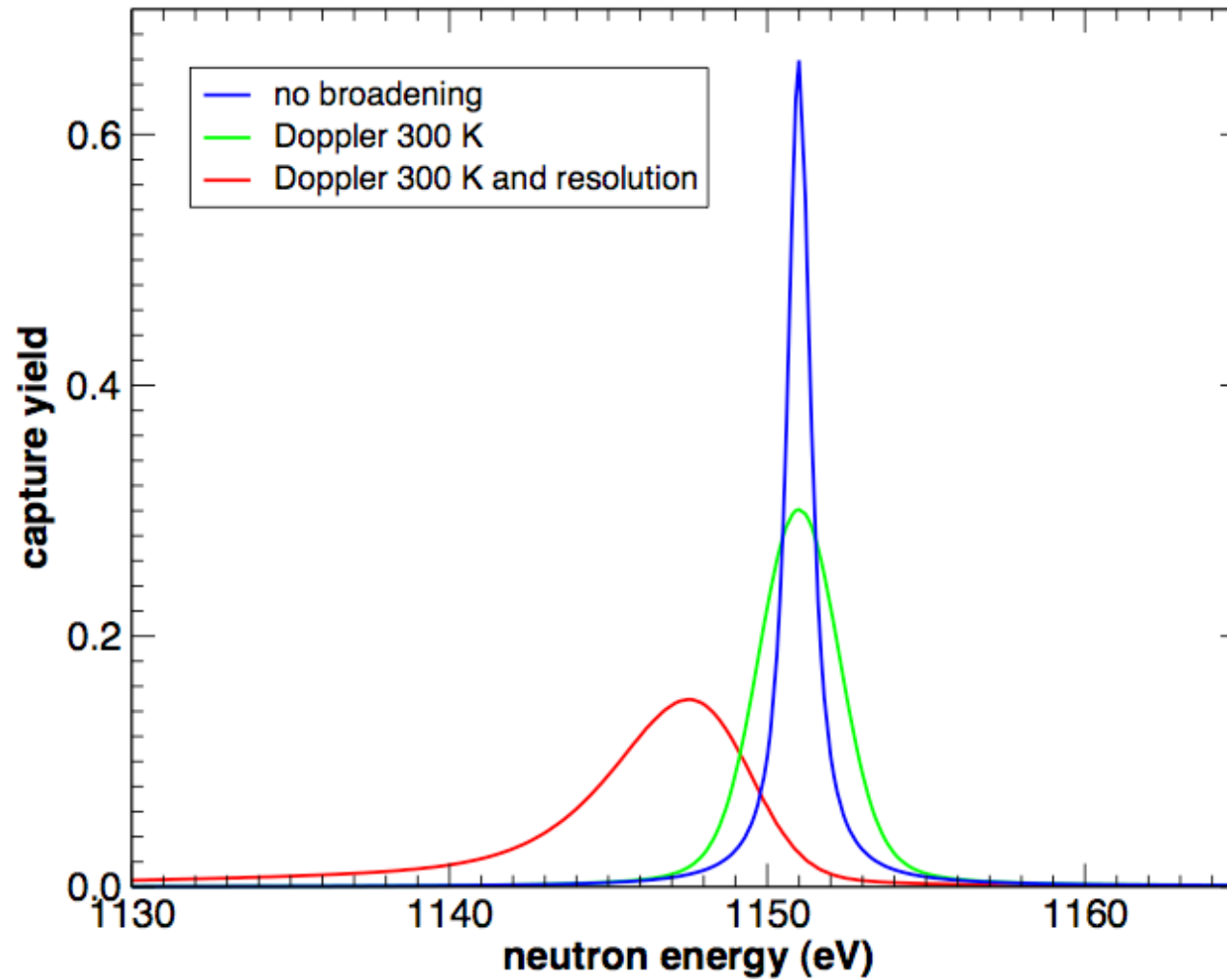
$$J^\pi, \ell, (g)$$

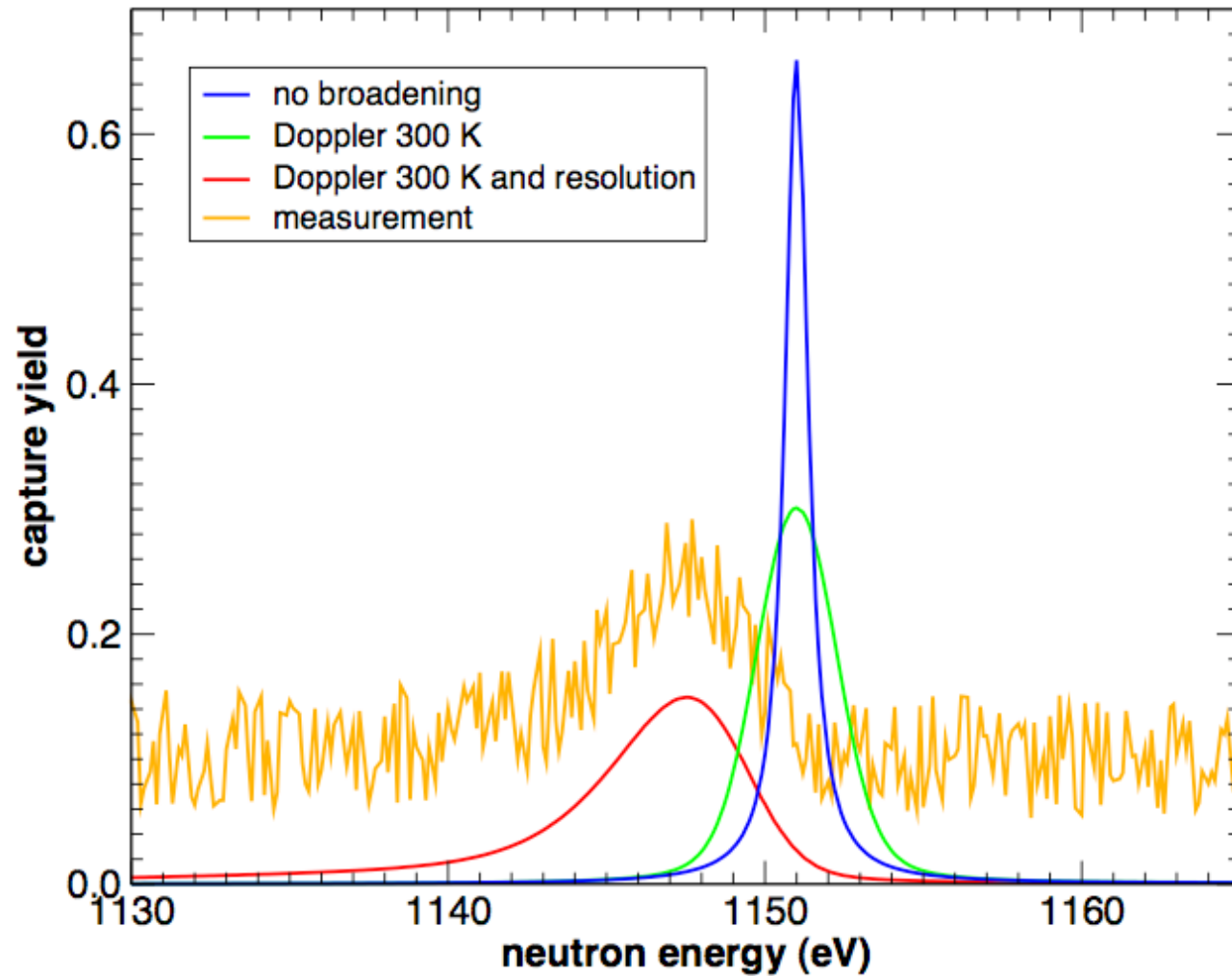
- cross sections at **300 K** (or any other temperature) include Doppler broadening
 - is a **solid state effect**, needs additional modelling and parametrization, at minimum temperature T . Simplest model: free gas
 - may also depend on material condition (crystal, powder, liquid, gas)
- cross sections are never measured experimentally, only reaction yields and transmission coefficients are obtained from measurements.
- experimental conditions include other models/parameters (resolution broadening, backgrounds)









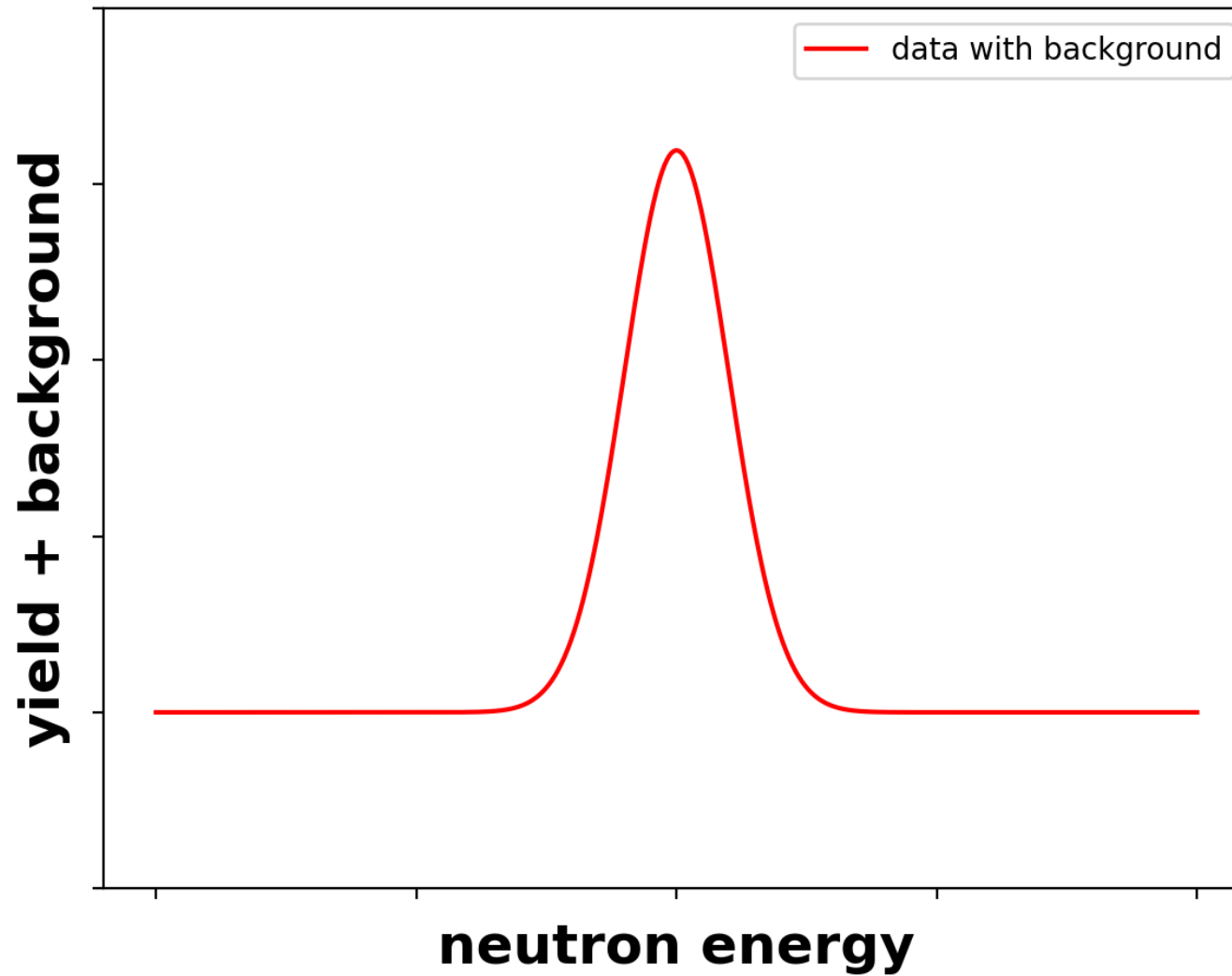


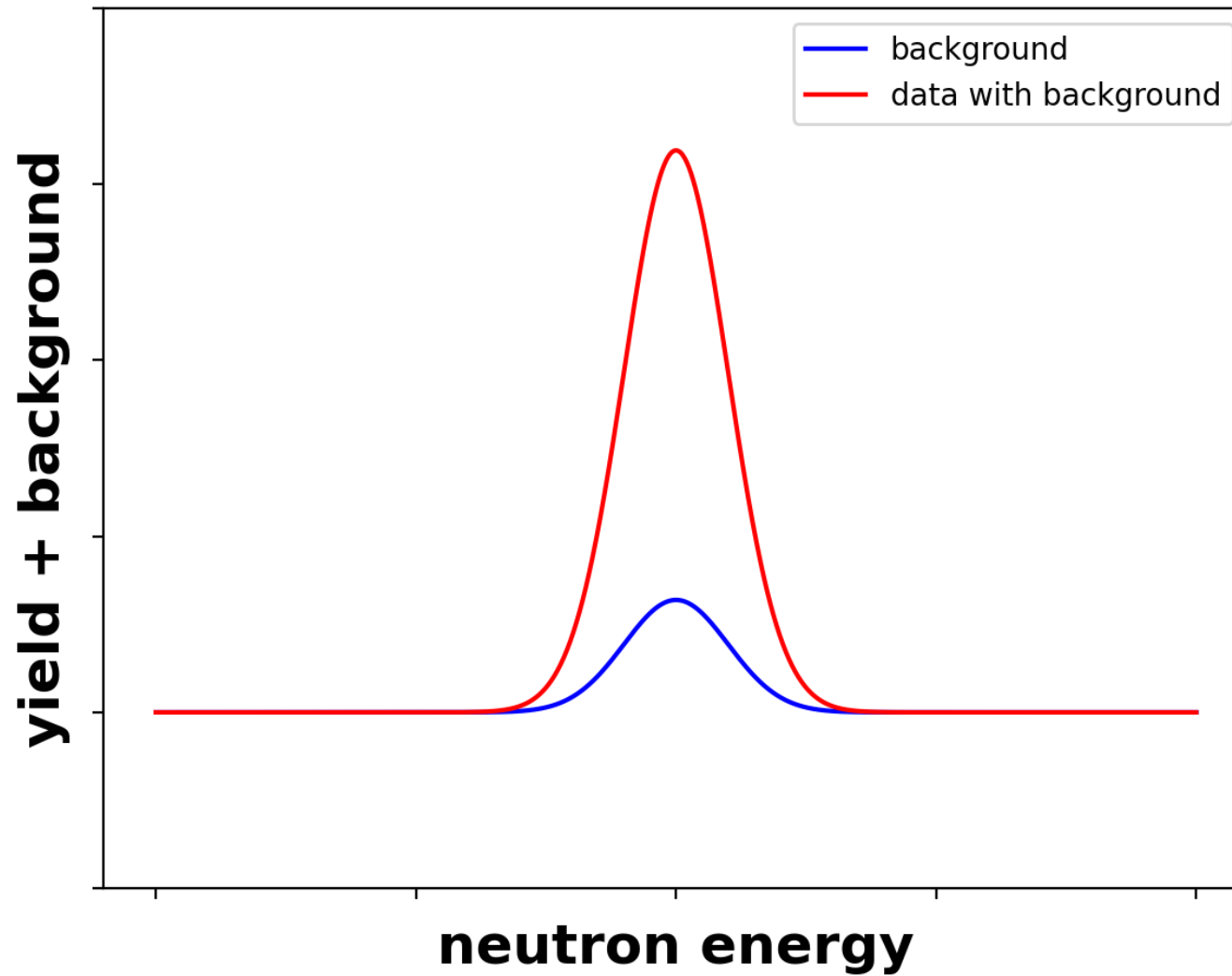
Fitting of Resolved Resonances

- Currently available codes: REFIT, SAMMY, (CONRAD)
- Fit of experimental data (chi-square minimization)
 - Non-linear fit: no guarantee to find global minimum.
 - Needs **initial values** as a starting point for minimization.
 - Different initial values may result in different local minima.
 - Mixture of discrete (spin, parity, orbital momentum) and continuous parameters.
 - Leaving many parameters free in a large energy range is results in non-optimal fits. Start with small energy ranges and optimize initial values. A global fit to obtain the covariance matrix should be done with close-to-final initial values.
In practice requires much user-interaction.
 - Use uncorrelated uncertainties of data points for fits.

Fitting of Resolved Resonances

- Backgrounds
 - Can be fitted for isolated resonances on a smooth background to obtain full covariances of parameters.
 - In case of overlapping resonances and for a smooth connection with the URR, background subtraction prior to fitting may be more accurate.
 - Background estimations are usually obtained from auxiliary measurements. Therefore background subtracted yields should be preferred.
 - Special attention is needed for backgrounds with the same shape as the resonance, i.e. resonance-scattered neutron backgrounds in capture yields.





Fitting of Resolved Resonances

- Experimental conditions
 - resolution (parametrized or numerical)
influences both widths and energy-calibration
 - multiple scattering in capture yields (scatter then capture)
 - detector efficiencies and angular distribution dependences
 - effects from sample shape, uniformity or granularity
- Bayesian fit or not
 - Informative priors are useful for evaluation production,
update of information while preserving existing covariance information
(sequential fit versus simultaneous fit)
 - Can be a problem for experimental analysis:
default priors can be too limited, default number of iterations too small
use uniform priors (standard maximum likelihood).
 - problem of a “non-converging” fit is often related to initial values, not to
broad priors.

