QENSmodels: Handling of units

At present the QENS models library contains a set of models aimed to fit S(Q, ħω) quasielastic neutron scattering data[1]. As there it does not yet exist an standard format for S(Q, ħω) data, it remains a user task to write the appropriate loader to read the data and the library is unit agnostic and it does not make any assumption about the units of the input data. As a consequence, if no additional information is given, any output parameter will be given in the same units as the input data. Further information and examples are given below.

S(Q, ħω)

The dynamical structure factor should be given in units of $[\text{energy}]^{-1}$ ($[E]^{-1}$), although in many cases S(Q, ħω) is not obtained in absolute units and the fitted data will be simply given in arbitrary units. In this case, the global scaling factor used in the fitting model will also be just an arbitrary number and its units can be ignored. Otherwise, if the input data were carefully normalized and the dynamical structure factor is given in absolute units, then this scaling factor will be given also in $[E]^{-1}$ units.

Q

The wavevector transfer has units of $[\text{length}]^{-1}$ ($[L]^{-1}$). Typically is given in $Å^{-1}$, but it is not strange to use nm^{-1} either.

ħω (or ω or ν or ν/c)

The energy exchange has naturally units of energy and it is commonly expressed in meV. However, many other units are also used in the literature. For example, for backscattering experiments it is quite usual to use μeV instead of meV. But it is also relatively frequent (especially when comparing with simulation data) to use just the angular frequency ω (often given in rad/ps or rad/s) or the frequency ν (often in THz, but also in GHz or Hz). In this case the input units are of dimension $[\text{time}]^{-1}$ ($[T]^{-1}$). Finally, in optical spectroscopy it is usual to use the optical wavevector ν/c in cm^{-1}, i.e. $[L]^{-1}$. Therefore it is not uncommon that neutron vibrational spectrometers provide data in cm^{-1}. However, as this is not of common use in QENS spectroscopy, we will not consider that case.

Output units

As said above, the units of the output parameters will correspond to the units of the input data. This implies that it remains the user responsibility to understand the nature of the parameters in each model in order to determine their units and then to convert the output values to any other physical unit[2]. A few examples to show how this can be done are given below.

Lorentzian or Gaussian models

Let's start with the most common case, where we fit a single Lorentzian and in the input data Q is given in $Å^{-1}$ and the energy transfer in meV. The three output parameters that we will get are the

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[1] In In the future the library could be extended to other types of models, e.g. inelastic or I(Q,t) models.

[2] As sometimes this can be confusing and a source of errors, we are working on implementing the possibility of declaring which are the units used in the input data and the desired units for the output data. Then the conversion will be done at the end of the fit and the final parameters given already in the units preferred by the user. TO DO!

amplitude of the Lorentzian: *scale*, given in arbitrary units (see above), its position: *center*, given in meV, and its half-width at half-maximum: *hwhm*, also given in meV.

It follows naturally that if the energy transfer is given in μeV, then *center* and *hwhm* will be returned also in μeV. And similarly if the input data contain S(Q, ω) or S(Q, ν) instead of S(Q, ħω) and the frequency is given in rad/ps or THz, respectively.

In this case, the standard unit conversion tables can be used to convert directly to the desired units, e.g.:

- List of conversion factors for neutron scattering
- Documentation about units in Mantid
- ILL online tool Neutron scattering conversion factors

The same applies to the Gaussian model, with *sigma* replacing *hwhm*.

Self-diffusion coefficient

Let's start with the simplest model, *Brownian Translational Diffusion.* This model has also three parameters. *Scale* and *center* will be treated as above. The third parameter is the self-diffusion coefficient, *D*, which is related to the half-width at half-maximum Γ of the Lorentzian function by the relation $\Gamma = DQ^2$. Thus $D = \Gamma/Q^2$ and its units will we $E\cdot L^2$ if the input data was S(Q, ħω) or $T^{-1}\cdot L^2$ if the input data was S(Q, ω) or S(Q, ν).

So if we fit S(Q, ħω) data with Q in $Å^{-1}$ and ħω in meV, D will be given in $Å^2$·meV. The output value can be converted to more standard units for the self-diffusion coefficient by noting that 1 Å = 10^{-10} m and ħω = 1 meV corresponds to ω = $1.519\cdot10^{12}$ rad/s, giving[3]:

$$1\ Å^2\cdot\text{meV} = 1.519\cdot10^{-8}\ m^2/s = 1.519\cdot10^{-4}\ cm^2/s = 1.519\ Å^2/ps$$

If the energy transfer is given in μeV instead of meV, then D will be obtained in $Å^2$·μeV, and we would need to apply:

$$1\ Å^2\cdot\mu\text{eV} = 1.519\cdot10^{-11}\ m^2/s = 1.519\cdot10^{-7}\ cm^2/s = 1.519\cdot10^{-3}\ Å^2/ps$$

If Q is in nm^{-1}, then we would have D in nm^2·meV or nm^2·μeV, and:

$$1\ nm^2\cdot\text{meV} = 1.519\cdot10^{-6}\ m^2/s = 1.519\cdot10^{-2}\ cm^2/s = 151.9\ Å^2/ps$$

$$1\ nm^2\cdot\mu\text{eV} = 1.519\cdot10^{-9}\ m^2/s = 1.519\cdot10^{-5}\ cm^2/s = 1.519\cdot10^{-1}\ Å^2/ps$$

If the input data correspond to S(Q, ω) with ω in rad/ps, then D will be obtained directly in $Å^2$/ps (if Q was in $Å^{-1}$) or in nm2/ps (if Q was in nm^{-1}).

Finally, if the input is S(Q, ν) with ν in THz and Q in $Å^{-1}$, then D will be in $Å^2$·THz, and:

$$1\ Å^2\cdot\text{THz} = 6.283\cdot10^{-12}\ m^2/s = 6.283\cdot10^{-8}\ cm^2/s = 6.283\cdot10^{-4}\ Å^2/ps$$

[3] Conversions done using the values appearing in the NIST conversion table.

Naturally, the same unit conversions can be applied to the parameter *D* in the Chudley-Elliot, jump translational diffusion, or the Gaussian localized diffusion models or in any other derived model where D represents a translational diffusion coefficient.

Distance parameters (e.g. jump length or radius)

They appear in many models, e.g. *L* in the Chudley-Elliot model for translational diffusion, or *radius* in the models of jumps among equivalent sites in a circle (simple or including a log-norm distribution) and isotropic rotational diffusion. They are in units of [L], i.e. the inverse of the units of Q, so if the input contains Q in $Å^{-1}$, then the output will be the length or radius in Å, while if Q was given in nm^{-1}, they will be returned in nm.

The same applies to the parameter $\langle u_x^2 \rangle$, quantifying the size of the region in which the particle is confined in the Gaussian model for localized diffusion[4]. In this case, $\langle u_x^2 \rangle$ is in units of L^2, so typically the parameter returned by the model will be in Å2 (if Q was in $Å^{-1}$) or in nm2 (if Q was in nm^{-1}).

Time parameters

At present, the only time parameter appearing in the library models is the residence time in a given site, called *resTime* in the jump translational diffusion and jump between equivalent sites in a circle (both simple or using a log-norm distribution or residence times) models. Its natural unit is T, of course, but if the input data correspond to S(Q, ħω), the resulting residence time will be given in E^{-1} units.

Therefore, in the most common case where we have experimental data with the energy transfer given in meV, the fit will give us a residence time τ in meV^{-1} which can be easily transformed to time units:

$$1\ meV^{-1} = 6.583 \cdot 10^{-13}\ s = 0.6583\ ps$$

Rotational diffusion coefficient

At present, this parameter appears only in the isotropic rotational diffusion model, named as *DR* and it will have units of E or directly T^{-1} if the input is S(Q, ω) instead of S(Q, ħω). In the first case, the result can be converted to the expected inverse time units easily:

$$1\ meV = 1.519 \cdot 10^{12}\ s^{-1} = 1.519\ ps^{-1}$$

Adimensional parameters

Although they do not require any conversion, they are listed here for completeness.

A0, *A1*, *A2* in models formed by the sum of several functions (e.g. delta_lorentz).

Nsites defining the number of sites in a circle (which should not be an adjustable parameter) in equivalent_sites_circle and jump_sites_log_norm_dist.

Sigma describing the width of the log-norm distribution in jump_sites_log_norm_dist

[4] F. Volino, J.-C. Perrin, and S. Lyonnard, *J. Phys. Chem. B* **110**, 11217-11223 (2006).