

OECD/NEA Meeting: WPEC SG38

“Beyond the ENDF Format: A Modern Nuclear Database Structure”

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Observations Related to Thermal Neutron Scattering Law Data

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Thermal Neutron Scattering

Using Born approximation, it can be shown that the double differential scattering cross section has the form

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{1}{4\pi} \frac{k'}{k} \left\{ \sigma_{coh} S(\vec{k}, \omega) + \sigma_{incoh} S_s(\vec{k}, \omega) \right\}$$

The scattering law $S(\vec{k}, \omega)$ is composed of two parts

$$S(\vec{k}, \omega) = S_s(\vec{k}, \omega) + S_d(\vec{k}, \omega)$$

Van Hove's formulation

$$I(\vec{k}, t) = \int G(\vec{r}, t) \exp(i\vec{k} \cdot \vec{r}) d\vec{r}$$

$$S(\vec{k}, \omega) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} G(\vec{r}, t) e^{i(\vec{k} \cdot \vec{r} - \omega t)} d\vec{r} dt$$

where $G(r,t)$ is the *dynamic pair correlation function* and is expressible in terms of the atomic positions.

Observations

1. S , the dynamic structure factor (or the scattering law), is a property of the scattering system and depends on the relative positions and motion (trajectories) of the atoms.
 - Atomic trajectories depend on the forces between atoms and temperature
2. S is completely independent of the neutron. It has nothing to do with the neutron energy, mass, etc.
3. This representation of scattering applies to thermal neutrons and other types of radiation (e.g., X-rays, electrons). However, in the case of neutrons the dynamics of system are sampled.

Observations

4. Low energy (thermal) neutrons have energies on the order of excitations in condensed matter and wavelength on the order of atomic distance.
 - This allows sampling the dynamics of the atomic system
5. An incoming neutron with such energies will sample S space according the usual conservation principles
 - Conservation of energy
 - Conservation of momentum

Discussion and Comments

Discussion point:

It was felt ... that we should consider focusing on storing possibly $\rho(\omega)$ and defer all subsequent discussions until the formation of a special WPEC subgroup that can specifically deal with TSL issues

Discussion and Comments

Discussion point:

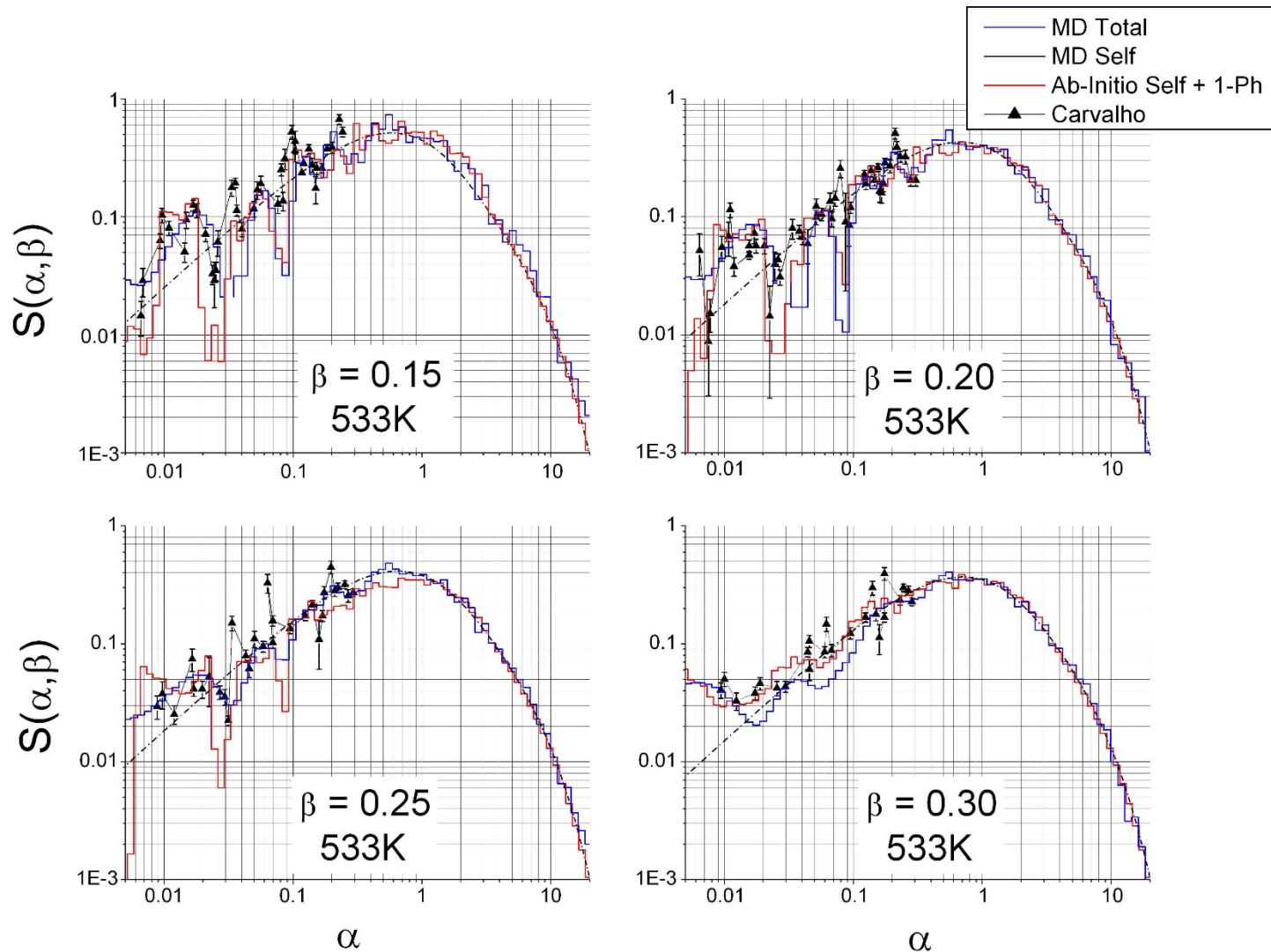
Reaction annotation could be used to split the scattering kernel into “self” and “distinct” parts. This is useful for a model-based evaluation where both components can be computed separately.

Comments:

Consider the end user of the data

- General user: only needs S (no concern about “self” and “distinct” components)
- Evaluator: may be interested in both components

Graphite Scattering Law



Discussion and Comments

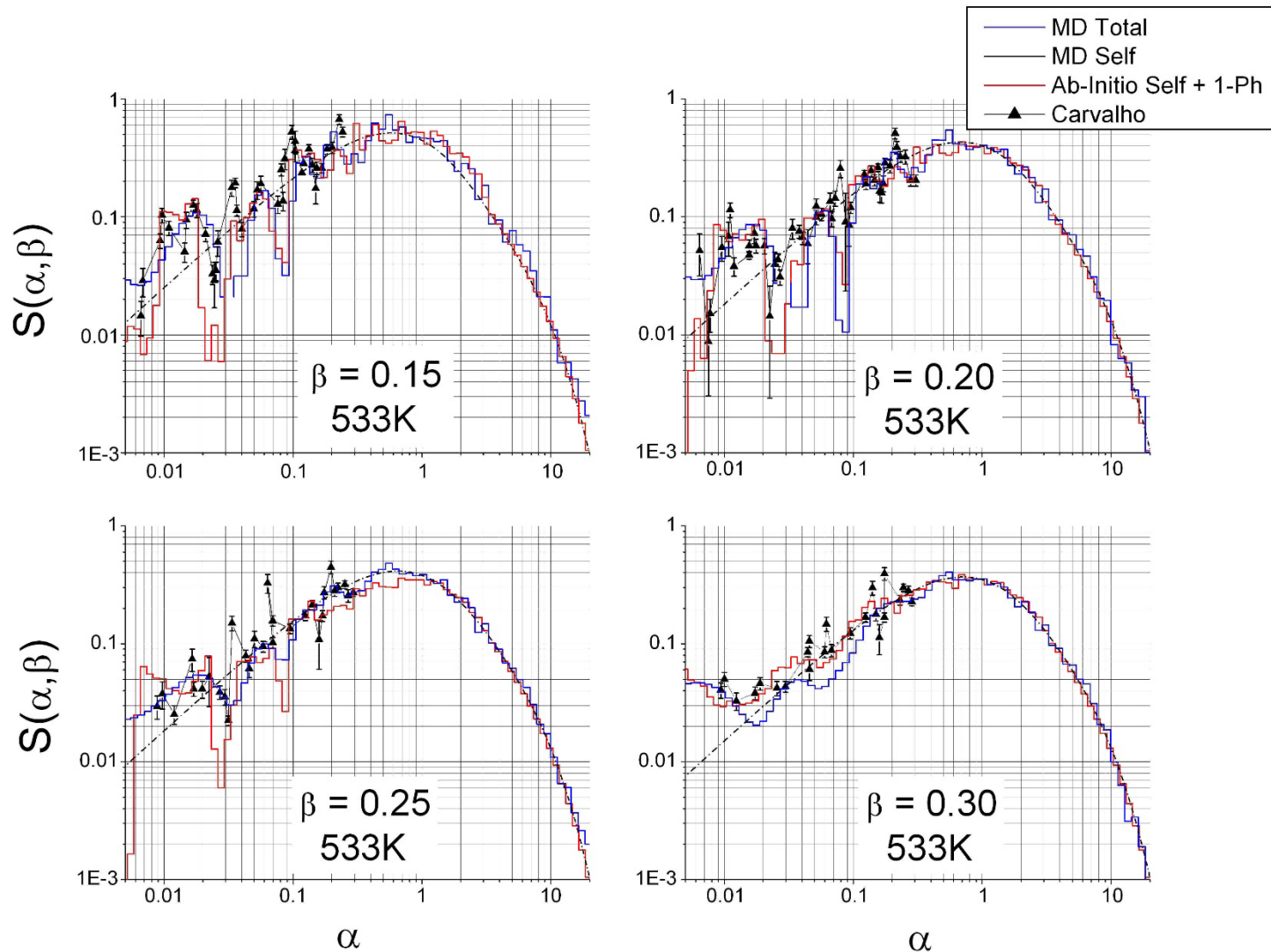
Discussion point:

New experiments from NCSU/RPI/ORNL collaboration will directly measure $d^2\sigma(E)/dE'd\Omega$. This is equivalent to measuring the full scattering kernel. Storing the covariance on the full scattering kernel may be unfeasible. Storing the covariance on data using the approximations and distinctions below may be feasible.

Comments:

- Scattering kernels can be calculated for all physical conditions of interest (temperature, pressure, etc.). Confirmation measurements for selected cases may be performed.
- Evaluators should assess covariance information for calculated and measured data separately to explore bias effects.

Graphite Scattering Law



Discussion and Comments

Discussion point:

ENDF thermal scattering data have a large dynamical range... Should we preserve this capability (SCT and store $\rho(\omega)$ directly) or store the $d\sigma(E)/dE'd\Omega$ directly, avoiding these precision problems?

Comments:

- Modern double precision capabilities make such issues less relevant. Even the “asymmetric” $S(\alpha, \beta)$ can be easily stored.
- Approximations such as SCT are also no longer relevant.

Discussion and Comments

Discussion point:

Denote the energy range for which these data are used. The $E_{max}=5$ eV limit in ENDF is convention and has no general physics justification.

Comments:

E_{max} is possibly a user issue as it can be treated as a material dependent parameter.