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Integrated intensities in inverse time-of-flight technique

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Abstract

In traditional data analysis a model function, convoluted with the resolution, is fitted to the measured data. In case that integrated intensities of signals are of main interest, one can use an approach which does not require a model function for the signal nor detailed knowledge of the resolution. For inverse TOF technique, this approach consists of two steps: (i) Normalisation of the measured spectrum with the help of a monitor, with $1/k$ sensitivity, which is positioned in front of the sample. This means at the same time a conversion of the data from time of flight to energy transfer. (ii) A Jacobian [I. Waller, P.O. Fröman, Ark. Phys. 4 (1952) 183] transforms data collected at constant scattering angle into data as if measured at constant momentum transfer Q. This Jacobian works correctly for signals which have a constant width at different Q along the trajectory of constant scattering angle. The approach has been tested on spectra of Compton scattering with neutrons, having epithermal energies, obtained on the inverse TOF spectrometer VESUVIO/ISIS. In this case the width of the signal is increasing proportional to Q and in consequence the application of the Jacobian leads to integrated intensities slightly too high. The resulting integrated intensities agree very well with results derived in the traditional way. Thus this completely different approach confirms the observation that signals from recoil by H-atoms at large momentum transfers are weaker than expected.

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1. Introduction

Pulsed spallation sources, such as ISIS in Great Britain, provide a high flux of epithermal neutrons up to several hundreds of electron volt. These high energy neutrons are needed for deep inelastic neutron scattering (DINS) which may also be called Compton scattering with neutrons. The inverse time-of-flight (TOF) instrument VESUVIO at ISIS is an instrument, unique in the world, for DINS. Since several years experiments with VESUVIO on H-containing materials [1] revealed that the signals from recoil by the H-atoms were weaker than theoretically expected.

In this context the data analysis procedure on VESUVIO has been questioned by Dawidovski et al. [2] and by Cowley [3]. These questions have been refuted by Mayers and Abdul-Redah [4]. In this paper we outline a new approach to derive integrated intensities for signals obtained in inverse TOF technique. As will be shown, this new approach agrees with the proposition made by Cowley [3] and also confirms the validity of the data analysis procedure used on VESUVIO.

Section 2 gives a very condensed review of the normalisation of the resolution function [5]. The performance of a monitor with a $1/k$ sensitivity is explained in Section 3. Section 4 introduces the Jacobian by Walter and Fröman [7]. This Jacobian is explicitly and very generally derived for isotropic dispersion in Section 5. This Jacobian represents an approximation in Compton scattering with neutrons, see Section 6. Finally in Section 7 the successful analysis of real data is given.

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2. Normalisation of the resolution function

Very generally, the measured intensity I represents the scattering function $S(\mathbf{Q},\omega)$ convoluted with the resolution function R of the instrument,

$$I\{\mathbf{Q}_0(t_0,\varphi_0),\omega_0(t_0)\} = \int S(\mathbf{Q},\omega)R\{\mathbf{Q}-\mathbf{Q}_0(t_0,\varphi_0),\omega-\omega_0(t_0)\}\,\mathrm{d}\mathbf{Q}\,\mathrm{d}\omega. \quad (1)$$

Here t is the total flight-time from the source to the detector and φ is the scattering angle. The index "0" indicates the mean values at a given position of the instrument. With

$$\hbar\omega_0 = \frac{\hbar^2k_\mathrm{I}^2}{2m} - \frac{\hbar^2k_\mathrm{F}^2}{2m}; \quad Q_0^2 = k_\mathrm{I}^2 + k_\mathrm{F}^2 - 2k_\mathrm{I}k_\mathrm{F}\cos\varphi, \quad (2)$$

where m is the mass of the neutron and k_I, k_F the wavevectors of the neutron before and after scattering, respectively.

The integral over the resolution function can be written as [5]

$$\int R(\mathbf{Q},\omega)\,\mathrm{d}\mathbf{Q}\,\mathrm{d}\omega = V_\mathrm{I}\cdot V_\mathrm{F}, \quad (3)$$

where

$$V_\mathrm{I} = \int^{\Delta k_{\mathrm{I},x}\Delta k_{\mathrm{I},y}\Delta k_{\mathrm{I},z}} p(k_\mathrm{I})\,\mathrm{d}k_{\mathrm{I},x}\,\mathrm{d}k_{\mathrm{I},y}\,\mathrm{d}k_{\mathrm{I},z} = p(k_\mathrm{I})\frac{1}{t_\mathrm{I}^4}\Delta\Omega_\mathrm{I}\Delta t_\mathrm{I},$$

$$V_\mathrm{F} = \int^{\Delta k_{\mathrm{F},x}\Delta k_{\mathrm{F},y}\Delta k_{\mathrm{F},z}} p(k_\mathrm{F})\,\mathrm{d}k_{\mathrm{F},x}\,\mathrm{d}k_{\mathrm{F},y}\,\mathrm{d}k_{\mathrm{F},z} = p(k_\mathrm{F})\frac{1}{t_\mathrm{F}^4}\Delta\Omega_\mathrm{F}\Delta t_\mathrm{F}, \quad (4)$$

where $t_\mathrm{I} \sim 1/k_\mathrm{I}$ and $t_\mathrm{F} \sim 1/k_\mathrm{F}$. $p(k_\mathrm{I})$ describes the source spectrum in phase-space. For a source in thermal equilibrium it reads

$$p(k_\mathrm{I}) = \exp(-k_\mathrm{I}^2/k_\mathrm{T}^2),$$

where k_T corresponds to the temperature of the moderator.

For an ideal source of epithermal neutrons it reads

$$p(k_\mathrm{I}) = (1/k_\mathrm{I}^4).$$

For a real source of epithermal neutrons such as ISIS it was found [4]

$$p(k_\mathrm{I}) = (1/k_\mathrm{I}^{3.8})$$

and $p(k_\mathrm{F})$ describes the analyser and detector efficiencies.

Dividing Eq. (1) by $V_\mathrm{I}\cdot V_\mathrm{F}$ gives

$$I_\mathrm{norm}(\mathbf{Q}_0,\omega_0) = \frac{I\{\mathbf{Q}_0(t_0,\varphi_0),\omega_0(t_0)\}}{V_\mathrm{I}\cdot V_\mathrm{F}} = \int S(\mathbf{Q},\omega)\frac{R\{\mathbf{Q}-\mathbf{Q}_0(t_0\varphi_0),\omega-\omega_0(t_0)\}}{V_\mathrm{I}\cdot V_\mathrm{F}}\,\mathrm{d}\mathbf{Q}\,\mathrm{d}\omega. \quad (5)$$

I_norm represents then a spectrum as if measured with a normalized resolution function. It is very important to note that the normalization of the resolution function by $V_\mathrm{I}\cdot V_\mathrm{F}$ includes the conversion from time-of-flight "t" to energy transfer "ω". No further Jacobian is required! In other words I_norm is a function of $\mathbf{Q}_0$ and ω_0, where $\mathbf{Q}_0$ and ω_0 have to be calculated from t_0 and φ_0. Integrating Eq. (5) over $\mathbf{Q}_0$ and ω_0 gives

$$\int I_\mathrm{norm}(\mathbf{Q}_0,\omega_0)\,\mathrm{d}\mathbf{Q}_0\,\mathrm{d}\omega_0 = \int S(\mathbf{Q},\omega)\,\mathrm{d}\mathbf{Q}\,\mathrm{d}\omega\cdot\text{constant}. \quad (6)$$

This fundamental relation, Eq. (6), can be used to obtain measured integrated intensities which correspond to the integral over a signal in $S(\mathbf{Q},\omega)$. The path of the integral in $\mathbf{Q}$–ω space can be $\mathbf{Q} = \text{constant}$, $\varphi = \text{constant}$ or any other. Integrals at $\mathbf{Q} = \text{constant}$ are often preferred, because theoretical expressions for $S(\mathbf{Q},\omega)$ are available at $\mathbf{Q} = \text{constant}$.

In the case of Compton scattering with neutrons, in the impulse approximation, the scattering function reads [6]

$$S(Q,\omega) = (\pi\Delta^2)^{-1/2}\exp\left\{-\left(\omega-\frac{Q^2}{2M}\right)^2\Big/\Delta^2\right\}, \quad (7)$$

where Δ is equal to Q times the momentum distribution of the initial states projected onto $\mathbf{Q}$. M is the mass of the recoiling atom. Eq. (7) is a normalised function at $Q = \text{constant}$.

3. A monitor with 1/k sensitivity

Going back to Eq. (5), in inverse TOF technique V_F is constant. V_I can be measured by a monitor with a $1/k$ sensitivity in the incoming beam in front of the sample [5]. Therefore I_norm can then be obtained by dividing the measured intensity I point by point by the corresponding monitor counts. Note, if one uses a black detector at the sample position, one measures $k_\mathrm{I}\cdot V_\mathrm{I}$.

Such a monitor with $1/k$ sensitivity is used on VESUVIO. With the help of this monitor it has been observed [4] that $V_\mathrm{I} \approx k_\mathrm{I}^{0.2} \approx E_\mathrm{I}^{0.1}$. Therefore on VESUVIO, $I_\mathrm{norm}(Q_0,\omega_0)$ is obtained by dividing the measured spectrum by $k_\mathrm{I}^{0.2}$ and by calculating Q_0 and ω_0 from t_0 and φ_0.

In practice it is convenient to consider $I_\mathrm{norm}(\varphi_0,\omega_0)$, the measured spectrum versus energy transfer ω_0 at constant scattering angle φ_0 but then care has to be taken to derive the integrated intensity, say of a Compton scattering signal.

4. The Jacobian by Waller and Fröman

The measured intensity of an excitation which is given by a dispersion relation $\omega(\mathbf{q})$ depends on the geometry in which the trajectory of the instrument $T(\mathbf{Q}_0,\omega_0)$ crosses the dispersion sheet $\omega_j(\mathbf{q})$ of mode j. $\mathbf{q}$ is the wavevector of the excitation in a Brillouin zone starting from its center $2\pi\boldsymbol{\tau}$. This problem has been studied by Waller and Fröman [7]. They write $S(\mathbf{Q},\omega)$ in the following way (somewhat modernised):