# CONSTANT-Q CONFIGURATION OF 3-AXIS SPECTROMETER

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## ABSTRACT

**CONSTANT-Q CONFIGURATION OF 3-AXIS SPECTROMETER**. The constant-*q* method has been widely used in the 3-axis spectrometer, which requires more angles to be setup as compared to those of the diffractometer. Those angles are not natural variables in the physical quantities of interest for the dynamic properties of materials. As the physical quantities of interests are the energy and momentum transfer, those angles must be converted into the energy and momentum transfer. To the author's knowledge, although this method has been known since around 1960's, no literature sufficiently describes the details to provide the necessary equations. This paper elaborates the conversion by using the energy and momentum conservation with the vector and trigonometric consideration of the scattering processes in the reciprocal space. The angle values resulted from this conversion might be used to obtained the dispersion relation measurement by utilizing the 3-axis spectromenter.

***Key words*** : Constant-Q, 3-axis spectrometer

## ABSTRAK

**KONFIGURASI Q-KONSTAN SPEKTROMETER 3-SUMBU.** Metode *q*-konstan telah banyak digunakan untuk spektrometer 3-sumbu, yang membutuhkan lebih banyak sudut pengukuran dibandingkan dengan sudut yang ada pada difraktometer. Sudut-sudut tersebut bukan merupakan variabel alamiah untuk besaran fisis sifat dinamika bahan. Karena besaran fisis tersebut adalah transfer energi dan momentum, sudut-sudut tersebut harus dikonversikan menjadi transfer energi dan momentum. Sepengetahuan penulis, walaupun metode ini sudah dikenal sejak sekitar tahun 1960-an, tidak ada literatur yang membahas secara rinci untuk menghasilkan persamaan yang diperlukan. Artikel ini mengupas konversi tersebut dengan menggunakan kekekalan energi dan momentum dengan pertimbangan vektor dan trigonometri dari proses hamburan di ruang kisi balik. Nilai-nilai sudut yang dihasilkan dalam konversi ini dapat digunakan untuk memperoleh pengukuran hubungan dispersi dengan menggunakan spektrometer 3-sumbu.

***Kata kunci*** : Q-Konstan, spektrometer 3-sumbu

## INTRODUCTION

A 3-Axis Spectrometer (TAS) is an indispensable tool to microscopically probe a dynamic properties of materials based on the momentum and energy conservation [1-5]. The dynamics properties of interest might consist of molecular vibrations and motions, coherent modes in glasses and liquids, lattice vibrations and anharmonicity, metallurgical systems, membrane proteins, crystal and magnetic structures, amorphous systems, spin waves, critical scattering, aggregate motions of polymers and biological systems. TAS has been installed at the Neutron Scattering Laboratory, BATAN, since 1992. However, the control and data acquisition system have been nonfunctional since 1996. It was difficult to fix the problem due to insufficient service manuals for such a complex instrument. TAS has 18 stepper motors to move the monochromator, the sample table and the analyzer axes equipped with the air compressor system to facilitate the movements of the massive axes.

Recently, as a part of in-house development of the neutron scattering facilities, an alternative control and data acquisition hardware have been developed by using local electronic parts. All motors can now be moved to specified positions as before but now with the know-how added value. The knowledge would ease further development and/or maintenance when necessary. This paper elucidates a constant-*q* measurement mode developed by a co-winner of the nobel prize, Brockhouse [1], which enables a measurement of the dynamics of the materials in a natural variable, i.e.; energy and momentum transfer experienced by the neutron beam scattered from the sample of interest. Although the constant-q technique has been widely used, there is no literature that provides the detail

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equations needed to describe the scattering configuration in the reciprocal space. This paper elaborates the scattering configuration in the reciprocal space, which is useful to automate the control and data acquisition of the dispersion relation from the neutron 3-axis spectrometer.

## TRIPLE AXIS SPECTROMETER

TAS consists of a monochromator, a sample table and an analyzer axes as shown in Figure 1. Neutrons of a defined wavelength are selected from the "white" beam by means of a single crystal monochromator (first axis). The wavelength or incident energy of neutrons depends on the monochromator material and the monochromator scattering angle $2\theta_M$. The sample diffracts by an angle $2\theta_S$ (second axis). The scattered neutrons are further analyzed with regard to their energy (third axis) by the analyzer via further diffraction process by an angle $2\theta_A$ and finally counted by the detector. The scattering vector **Q** and the energy transfer ΔE are unequivocally determined by the angle $2\theta_S$ and $2\theta_A$. Thereby, the wave vectors $\mathbf{k}_i$ and $\mathbf{k}_f$ are connected with vector **Q** and energy transfer by $\mathbf{Q}=\mathbf{k}_i-\mathbf{k}_f$ and $\Delta E= h^2(k_i^2-k_f^2)/(2m)$. The sense of the energy transfer determines whether the neutron has gained ($k_i<k_f$, $\Delta E<0$) or lost energy ($k_i>k_f$, $\Delta E>0$) during the scattering process.

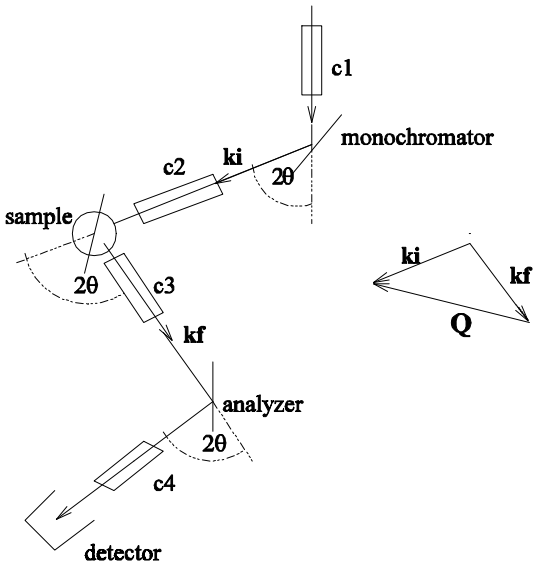


***Figure 1.*** A schematic of BATAN 3-axis spectrometer. The beam of interest comes before the collimator c1. The vector triangle connecting $k_i$, $k_f$ and Q is shown in the right-side.

It is possible to operate with a very flexible unit allowing automatic changes of the scattering angle $\phi=2\theta_S$, the crystal direction ψ, the magnitude of the incident wave vector $k_i$ related to the monochromator scattering angle $2\theta_M$ and the magnitude of the scattered wave vector $k_f$ related to the analyzer scattering angle $2\theta_A$. Those changes can be triggered, at the end of any counting period, according to suitable pieces of information coming in general, from a computer. The control and data acquisition program codes, as shown in Figure 2, have been developed using GNU C++ programming language with visual capabilities provided by wxWidgets [6]. The GNU C++ and wxWidgets are available freely from the internet and of good quality which also enable source code platform independent.

## ELASTIC SCATTERING CONFIGURATION IN RECIPROCAL SPACE

Figure 2 shows elastic measurement mode in various equivalent configurations to provide a clear connection between the elastic and inelastic scattering configuration. Figure 2(a) is usually the most common way to describe the diffraction configuration. The incident beam, with the propagation vector $\mathbf{k}_i$, comes into the sample and is scattered with the scattering angle ϕ. Figure 2(b) is the transition between the most common way to the figure usually used in the inelastic scattering. Unlike Figure 2(a), Figure 2(b) shows the opposite of the scattered propagation vector $\mathbf{k}_f$. Without changing the magnitude, ϕ is now the angle between $\mathbf{k}_i$ and $-\mathbf{k}_f$. In Figure 2(c), the sample marker is shifted into the origin of the scattering coordinates. Although Figure 2 belongs to the elastic scattering in which $|\mathbf{k}_i|=|\mathbf{k}_f|$, Figure 2(c) can easily be generalized to the inelastic case in which $|\mathbf{k}_i|\neq|\mathbf{k}_f|$.

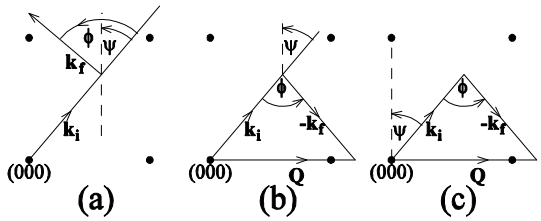


***Figure 2.*** Elastic measurement mode shown in various equivalent configurations. Dots indicate constructive interference in the reciprocal space, which are usually indexed by the Miller indices. Dashed lines indicate the reference of the crystal orientation. The crystal direction and the scattering angle are denoted as ψ and ϕ, respectively.

Some remarks are in order. Firstly, it is a common practice to choose the scattering vector **Q** as $(\mathbf{k}_i - \mathbf{k}_f)$. This choice relates to the negative of the Miller indices, instead of the positive ones. Most literatures do not put the minus sign in the Miller indices as the positive and the minus indices are the Friedel pairs, which has the equivalent intensities. Secondly, one might choose **Q** as $(\mathbf{k}_f - \mathbf{k}_i)$. In this choice, ψ relates the crystal direction and $(-\mathbf{k}_i)$, instead of $\mathbf{k}_i$. The relation to the negative direction of the incident propagation vector instead of the positive one makes the configuration a little more difficult. Thirdly, in both choices, one must note that the energy transfer, which is useful for the inelastic

scattering to be discussed below, is always expressed as the final neutron energy minus the initial neutron energy. It is not expressed in the other way around. Fourthly, the momentum transfer related to the non-zero scattering angle is non-zero for both the elastic and inelastic scattering. However, the energy transfer is only non-zero for the inelastic scattering.

## INELASTIC SCATTERING CONFIGURATION IN RECIPROCAL SPACE

The governing equations for the 3-axis mode are the energy and momentum conservations. With the energy conservation, one can choose to fix either the incident or the scattered neutron wavelength. In principle, there are two modes related to the wave propagation vector, i.e. the longitudinal and the transversal. In the longitudinal and transversal mode, the relation between the wave polarization vector and the propagation vector is parallel and perpendicular, respectively. With the momentum conservation, one can choose to search either longitudinal, transversal mode, or both modes of the phonon vibration. One usually restricts the situation into the longitudinal or the transversal by choosing appropriate measurement in the high symmetry point in crystal. Figure 3 details the situation for the longitudinal mode (Figure 3(a) and (c)) and the transversal mode (Figure 3(b) and (d)). The axes in Figure 3(a) and (c) (and subsequently in Figure 3(b) and (d)) are chosen to provide the unique axes of high symmetry in the reciprocal lattice. For example, in the simple cubic crystallographic structure, one can choose (100) and (011) as the horizontal and vertical axes.

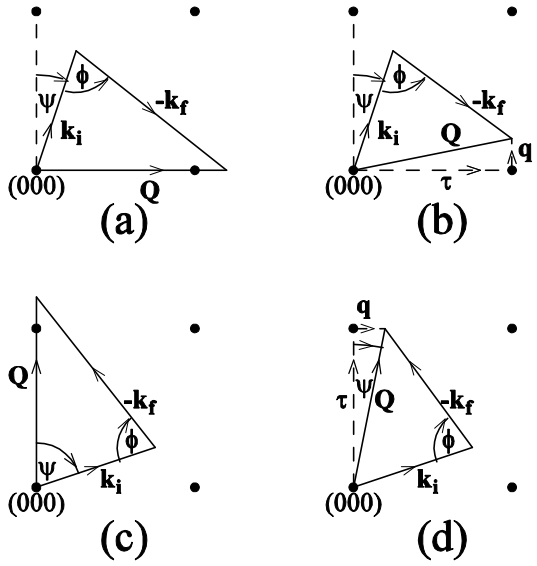


***Figure 3.*** Measurement configurations in reciprocal space for the longitudinal mode (Figure (a) and (c)) and (Figure (b) and (d)) showing the scattering angle $\phi$ and the incident beam to crystal direction $\psi$, related to the scattering vector Q, the incident wavenumber vector $k_i$ and the scattered wavenumber vector $k_f$.

In all cases shown in Figure 3 with the incident wavenumber $k_i=2\pi/\lambda_i$, the scattered wavenumber $k_f=2\pi/\lambda_f$ and scattering vector $\mathbf{Q}=\boldsymbol{\tau}+\mathbf{q}$; the scattering angle $\phi$ can be obtained from

$$\phi = \pm \arccos\left(\frac{k_i^2 - k_f^2 - Q^2}{2k_i k_f}\right) \quad \text{..... (1)}$$

The crystal directions $\psi$ for Figure 3(a) and (c), respectively, are determined by:

$$\psi_a = \frac{\pi}{2} - \arccos\left(\frac{k_i^2 + Q^2 - k_f^2}{2k_i Q}\right) \quad \text{..... (2)}$$

$$\psi_c = \arccos\left(\frac{k_i^2 + Q^2 - k_f^2}{2k_i Q}\right) \quad \text{..... (3)}$$

The formula for $\psi_b$ and $\psi_d$ are analogous to $\psi_a$ and $\psi_c$, respectively. To provide an appropriate offset value of $\psi$s, one can proceed further so that in the elastic regime, in which $k_f=k_i$ and hence Braggs law is satisfied, we have $\psi^{elastic}=\phi/2$. This relation can be obtained either from the hardware setup, i.e.; by appropriately defining the zero of $\psi$ or from the software calculation.

Albeit their simplicities, Eq. (2) and (3) are not easily generalized to automate the data acquisition. To separate the longitudinal and transversal phonon measurement using one formula, the scattering vector **Q** must be expressed in terms of their Cartesian components. One then resorts to vector consideration in addition to the trigonometric relations. One can start by taking the Cartesian components of the scattering vector $\mathbf{Q}=\mathbf{k}_i-\mathbf{k}_f$. By simple trigonometric manipulations on the Cartesian components $Q_x$ and $Q_y$, one has:

$$Q_x = k_i \sin\psi - k_f \sin(\phi - \psi) \quad \text{..... (4)}$$

$$Q_y = k_i \cos\psi + k_f \cos(\phi - \psi) \quad \text{..... (5)}$$

which can readily be written as:

$$k_f \sin(\phi - \psi) = k_i \sin\psi - Q_x \quad \text{..... (6)}$$

$$k_f \cos(\phi - \psi) = Q_y - k_i \cos\psi \quad \text{..... (7)}$$

Squaring Eq. (6) and (7), and adding them up, one has

$$Q_x \sin\psi + Q_y \cos\psi = \frac{Q^2 + k_i^2 - k_f^2}{2k_i} \quad \text{..... (8)}$$

Dividing both sides of Eq. (8) by $\cos\psi$, using the trigonometric relation $\cos\psi = (1 + \tan^2\psi)^{-1/2}$ and squaring both sides of the resulted equation yield

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$$\left(Q_x^2 - A^2\right)\tan^2\psi + 2Q_xQ_y\tan\psi + Q_y^2 - A^2 = 0 \quad \text{..... (9)}$$

where

$$A = (Q^2+k_i^2-k_f^2)/(2k_i) \quad \text{..... (10)}$$

The solutions are:

$$\psi_{\pm} = \arctan\left(\frac{-Q_xQ_y \pm A\sqrt{Q^2 - A^2}}{Q_x^2 - A^2}\right) \quad \text{..... (11)}$$

Some comments are in order. Firstly, one must note that Eq. (11) has multiple values. One particular value of the arctan argument corresponds to an angle of $(2\pi n+\alpha)$ and $(2\pi n+\pi+\alpha)$ where $n$ is any integer. This multiple value situation provides more choices of the angle setup to avoid possible orientation limitations. Secondly, as a quick check, one can take the elastic case in which the scattering vector Q lies at the horizontal axes such that Qy=0. In such case, $A=2\pi \sin(\theta)/d$ and

$$\psi_{\pm}^{elastic} = \pm\theta \quad \text{..... (12)}$$

as expected in the elastic scattering. Thirdly, as an alternative to solve Eq. (8), one can use any commercial software, such as Maple or Mathematica, to solve the equations automatically. However, the resulted expressions are much more cumbersome and the denominator of the arctan argument contains $Q_x$ factor which can be zero, and hence more ill-conditioned.

## CONCLUSIONS

The 3-axis spectroscopy allows the determination of the energy transfer by analysis of the wavelength. To achieve this, the neutrons are characterized before and after hitting the sample. Three processes (monochromatization, sample interaction and analyzing) make up the three axes of the 3-axis spectrometer.

The 3-axis spectrometer requires more angles to be setup as compared to those of the diffractometer. Those angles are not natural variables in the physical quantities of interest. As the physical quantities of interests are the energy and momentum transfers, those angles must be converted into the energy and momentum transfers. This has been done by using the energy and momentum conservations with vector and trigonometric consideration of the scattering processes in the reciprocal space. The angles resulted from this process might be used to obtained the dispersion relation curve.

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