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The effect of gravity on the resolution of small-angle neutron diffraction peaks

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The resolution ellipses for neutron diffraction peaks at small scattering vectors lie along lines that point to a position vertically above the beam center on the small-angle scattering detector. This gravity effect is only noticeable for neutron beams at long wavelengths and with large wavelength spreads.

It is well known that the neutron, with mass m, experiences a gravitational field and that a beam of thermal neutrons follows a parabolic path caused by the acceleration due to gravity g. McReynolds (1951) was the first to measure the influence of gravity on a thermal neutron beam. The effect is small and may be ignored in the vast majority of neutron scattering measurements. However, the use of both long-wavelength neutrons and long flight paths results in both the transmitted beam and the scattered neutrons falling by a measurable amount that is wavelength dependent. In the case of small-angle scattering, simple kinematics shows that the change Δy_g in the vertical height of a beam of neutrons of wavelength λ at the detector is given by

$$\Delta y_g = -L_2(L_1 + L_2)(g/2)(m/h)^2\lambda^2 = -A\lambda^2, \qquad (1)$$

where L_1 and L_2 are the distances between the source and sample apertures and the sample aperture and the detector, respectively, and h is Planck's constant. The neutron velocity is $h/m\lambda$. Furthermore, the wavelength spread of the incident beam causes vertical smearing of both the transmitted and the scattered beams. For a scattering function that has no azimuthal dependence for which the data can be radially averaged, the scattering angle and location on the detector vary with the incident wavelength. Consequently, with finite wavelength spread, the Debye–Scherrer ring is no longer circular but oval, with a broader vertical width at the bottom than at the top. Boothroyd (1989) has given an analytic form for the gravity resolution function for symmetric data when the beam center is not corrected for gravity. Barker & Pedersen (1995) have also developed corrections to the resolution function for symmetric data to account for gravity when the beam center corresponds to the mean wavelength.

Forgan & Cubitt (1998) have shown a diffraction pattern from a flux lattice in the low-T_c superconductor Nb with λ = 19.4 Å wavelength neutrons, with a wavelength distribution having a full width at half-maximum (FWHM) of $\Delta\lambda/\lambda$ = 10%. The shape of the diffraction spots is distorted by the combination of gravity and wavelength spread. Their figure shows that the diffraction peaks below the horizontal line through the instrument center line are elongated in the vertical direction, whereas those above are more circular. In fact, the wavelength contribution to the resolution is always in the direction of the scattering vector **Q** [$Q = (4\pi/\lambda)\sin(\theta/2)$, where θ is the scattering angle] and increases with its magnitude, whereas gravity is always in the vertical direction. They also show that the insertion of suitable prisms immediately before the sample can compensate for the distortion to the peaks caused by gravity.

In an effort to determine an analytic description of the resolution of azimuthally asymmetric scattering data, we have re-examined discarded data measured on single-crystal Nb more than ten years ago on the NG7 SANS instrument (Glinka *et al.*, 1998). Fig. 1 shows the diffraction from the flux lattice at a temperature of 6 K taken with 20 Å neutrons and a wavelength spread $\Delta\lambda/\lambda$ = 22%. The flight path lengths (L_1 = 15.77 m and L_2 = 15.85 m) give a value of A = 0.1564 mm Å^{-2}. The data show the elongation of the Bragg diffraction peaks. However, we notice that the major axes of the elliptical contours do not point towards the displaced beam center but to a position significantly above. This can also be observed in the data of Forgan & Cubitt (1998).

In the absence of gravity, the resolution of the vector $\mathbf{Q}_0$ located at (R, φ) on the detector, where R is the distance to the instrument center line and φ is the azimuthal angle relative to the horizontal, is

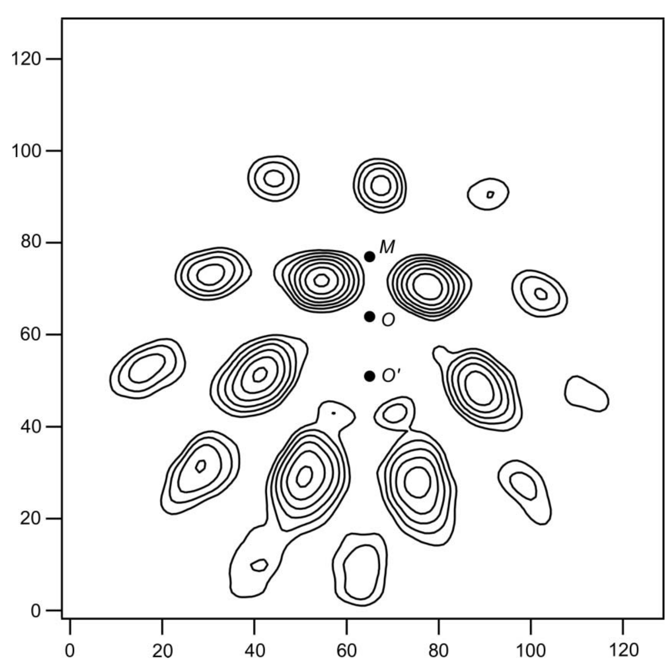

Figure 1
The diffraction pattern, showing the sixfold symmetry of the Bragg peaks from the vortex lattice of single-crystal Nb at T = 6 K, taken on beamline NG7 SANS at NIST with 20 Å neutrons and with a wavelength spread $\Delta\lambda/\lambda$ = 22%. The point O corresponds to the spectrometer axis and the point O' to the center of the diffraction pattern. The major axes of the diffraction spots tend to point towards M.

best expressed in directions along and perpendicular to the direction of the scattering vector (see Pedersen *et al.*, 1990). The resolution function of this vector **Q** measurement is

$$\Re(Q_0, Q_{||}, Q_{\perp}) = (2\pi\sigma_{Q_{||}}\sigma_{Q_{\perp}})^{-1}\exp\left[-(Q_{||}-Q_0)^2/2(\sigma_{Q_{||}})^2\right] \times \exp\left[-Q_{\perp}^2/2(\sigma_{Q_{\perp}})^2\right], \quad (2)$$

with values of the variances (Mildner & Carpenter, 1984) given by

$$(\sigma_{Q_{\perp}})^2 = \sigma^2_{\rm geom} = \frac{k^2}{12}\left[3\left(\frac{R_1}{L_1}\right)^2 + 3\left(\frac{R_2}{L'}\right)^2 + \left(\frac{\Delta d}{L_2}\right)^2\right],$$
$$(\sigma_{Q_{||}})^2 = \sigma^2_{\rm geom} + Q_0^2(\sigma_\lambda/\lambda)^2, \quad (3)$$

where the wave vector $k = 2\pi/\lambda$, $|\mathbf{Q}_0| = kR/L_2$ and σ^2_λ is the wavelength variance. R_1 and R_2 are the radii of the source and sample apertures, respectively, Δd is the size of the detector element or pixel, and $L'^{-1} = L_1^{-1} + L_2^{-1}$. Hence, in the absence of the gravity term or when it can be neglected, the resolution function of the vector **Q** is elliptical with its major axis along **Q** and pointing towards the origin, the beam center on the detector. We now show how this is different when gravity is taken into account.

Gravity causes the mean of the center of the beam to be displaced by $\Delta y_g = -A\langle\lambda^2\rangle$ relative to the instrument axis, where $\langle\lambda^2\rangle = \lambda_0^2[1 + (\sigma_\lambda/\lambda)^2]$ and λ_0 is the mean wavelength. This results in an extra spatial variance in the y direction of the incident beam, given by

$$\sigma_g^2 = A^2[\langle\lambda^4\rangle - \langle\lambda^2\rangle^2] = 4A^2\lambda_0^4(\sigma_\lambda/\lambda)^2. \quad (4)$$

If the incident beam has a triangular wavelength distribution FWHM of $\Delta\lambda$ around the mean wavelength λ_0, then the wavelength resolution is $(\sigma_\lambda/\lambda)^2 = (1/6)(\Delta\lambda/\lambda_0)^2$. Hence, $\sigma_g^2 = (2/3)A^2\lambda_0^4(\Delta\lambda/\lambda_0)^2$ must be added to the variance of the incident-beam width in the vertical direction (Mildner *et al.*, 2005). The upper edge of the beam, defined by the faster neutrons, moves down less than the lower edge, defined by the slower neutrons. The result is an oval shape or distortion of the incident beam on the detector. The magnitude of the scattering vector should be determined relative to this mean beam center, which is displaced by $-A\lambda_0^2$ from the instrument center line.

The centers of all the diffraction peaks are also displaced by the same amount $-A\lambda_0^2$ as the mean beam center. However, each diffraction spot has a different resolution ellipse. There is no wavelength component in the direction perpendicular to **Q**, and only the parallel component needs correction for gravity. The gravity contribution (along $\hat{\mathbf{y}}$, the unit vector in the vertical direction) to the uncertainty in **Q** is not independent of the wavelength contribution (which is in the direction of $\mathbf{Q}_0$). Hence, both contributions add as vectors to give the resultant variance $[\mathbf{Q}_0 - 2A\lambda_0^2(k/L_2)\hat{\mathbf{y}}]^2(\sigma_\lambda/\lambda)^2$. We may resolve the wavelength contribution into horizontal and vertical components, so that the overall wavelength contribution to the variance along the major axis becomes $(k/L_2)^2[R^2\cos^2\varphi + (R\sin\varphi - 2A\lambda_0^2)^2](\sigma_\lambda/\lambda)^2$, where φ is the azimuthal angle of the peak relative to the horizontal axis.

The resolution ellipse has its major axis along the line joining (R, φ) and $(2A\lambda_0^2, \pi/2)$ with a variance

$$(\sigma_{Q_{||}})^2 = \sigma^2_{\rm geom} + (1/6)(k/L_2)^2(\Delta\lambda/\lambda)^2[R^2 - 4RA\lambda_0^2\sin\varphi + 4A^2\lambda_0^4], \quad (5)$$

assuming a triangular wavelength distribution. The expression makes sense at various limits. If gravity is negligible ($A \simeq 0$), the variance for the wavelength spread is its usual value [equation (3)]. If there is no wavelength spread, there is no gravity component to the resolution, and therefore there is only geometric smearing. Finally, it gives the correct value for the incident beam (**Q** = 0). Note that the gravity-dependent terms in equation (5) normally increase the variance, but they can actually cancel all wavelength-dependent components at a position offset vertically from the beam center by $2A\lambda_0^2$, where the contours of a diffraction spot would appear circular.

Fig. 2 illustrates the above result graphically. Consider the scattering at a particular value of the scattering vector **Q**. Its location (R, φ) on the detector as a function of wavelength λ in the absence of gravity is determined by

$$|\mathbf{Q}| = k\theta = (2\pi/\lambda)(R/L_2) = (2\pi/\lambda)(y/\sin\varphi L_2). \quad (6)$$

The variation in the vertical coordinate Δy on the detector for the scattering vector **Q** is related to the wavelength variation $\Delta\lambda$ by $\Delta y/y_0 = \Delta\lambda/\lambda_0$, where y_0 is the vertical position for the mean wavelength λ_0 of the incident beam. In the absence of gravity, the major axis of the resolution function, which is determined by the wave-

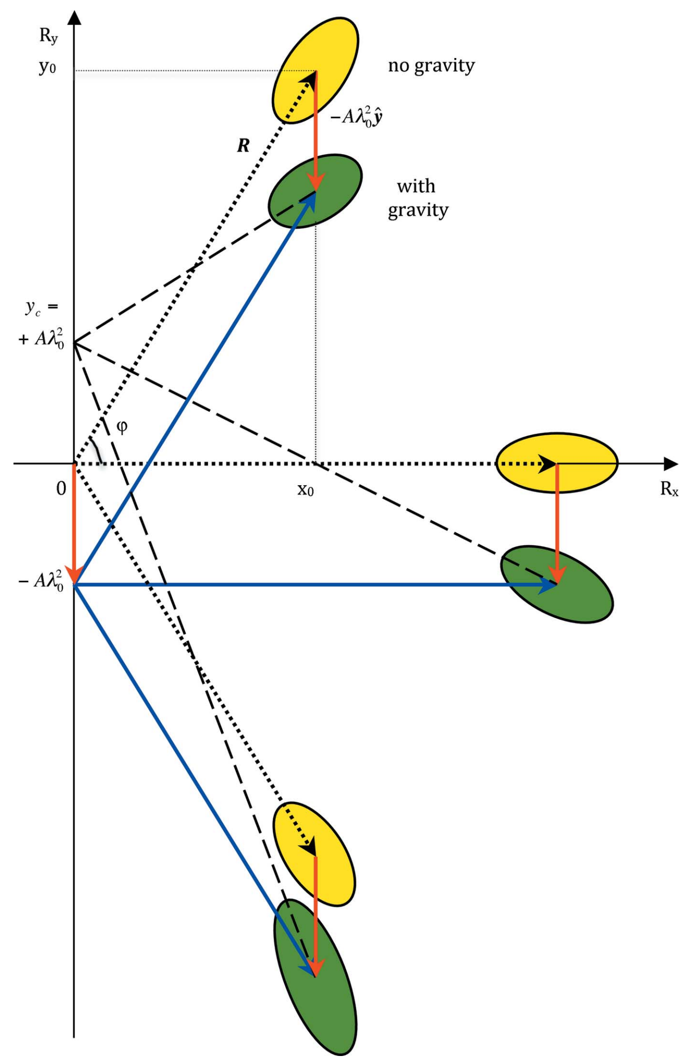

Figure 2
A schematic drawing showing the resolution ellipses for the diffraction spots in the cases of no gravity and with gravity. With no gravity, the major axis (dotted line) of the resolution ellipse for a scattering vector $\mathbf{Q}_0(R, \varphi)$ lies on a line through the origin (the instrument center line) with a gradient $\tan\varphi$. With gravity, the centers of all ellipses are displaced vertically by $-A\lambda_0^2$, with the vector **R** (solid line) measured relative to the displaced center $(0, -A\lambda_0^2)$, but the major axes of the resolution functions all point towards $(0, A\lambda_0^2)$ (dashed line). Gravity changes the direction of the major axes, and can either reduce or increase the variance in the major-axis direction.

length contribution, lies along a line through the origin in the direction of **Q** with a slope m' on the detector given by

$$m' = \tan\varphi = y_0/x_0 = \Delta y/\Delta x, \quad (7)$$

where $\Delta y/\Delta x$ is the gradient of the ellipse major axis at its center corresponding to λ_0.

In the presence of gravity, locations on the detector with different wavelengths and scattering angles that correspond to the same value of **Q** are each displaced vertically by a distance $-A\lambda^2$ rather than $-A\lambda_0^2$. That is, the major axis of the resolution function now lies along a line with slope m'' and intercept y_c on the detector given by

$$m'' = (y_0 - A\lambda_0^2 - y_c)/x_0 = \Delta(y - A\lambda^2)/\Delta x. \quad (8)$$

That is,

$$(A\lambda_0^2 + y_c) = 2A\lambda_0(\Delta\lambda/\Delta x)x_0 = 2A\lambda_0^2, \quad (9)$$

so that the intercept $y_c = A\lambda_0^2$ relative to the instrument center line as the origin, or $2A\lambda_0^2$ relative to the beam center line. Hence the lower diffraction spots are elongated, as shown in Fig. 1, and the upper spots are more circular. (Note that the major axis of the resolution ellipse is in fact curved, since the gradient of the major axis varies with λ and the y intercept varies with λ^2.)

The resolution ellipse is distorted when gravity is taken into account, with the major axis of the resolution function for a diffraction peak lying along a line that intercepts the y axis at a point $A\lambda_0^2$ relative to the instrument axis, where λ_0^2 is the mean-square wavelength for the distribution, even though the center of the incident beam on the detector lies at the vertical point $-A\lambda_0^2$. In general, both the mean wavelength λ_0 and the width $\Delta\lambda$ of the distribution are sufficiently small that this effect may in fact not even be noticed.

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