

1 **A super-resolution technique to analyze single-crystal inelastic neutron scattering**
2 **measurements using direct-geometry chopper spectrometers^{a)}**

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9 Direct-geometry time-of-flight chopper neutron spectroscopy is instrumental in studying
10 dynamics in liquid, powder, and single crystal systems. We report here that *real*-space
11 techniques in optical imagery can be adapted to obtain *reciprocal*-space super resolution
12 dispersion for phonon or magnetic excitations from single-crystal neutron spectroscopy
13 measurements. The procedure to reconstruct super-resolution energy dispersion of excita-
14 tions relies on accurate determination of the momentum and energy-dependent point spread
15 function, and a dispersion correction technique inspired by an image disparity calculation
16 technique commonly used in stereo imaging. Applying these methods to spinwave dis-
17 persion data from a virtual neutron experiment demonstrates ~ 5 -fold improvement over
18 nominal energy resolution.

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19 I. INTRODUCTION

20 Inelastic neutron scattering (INS) is a powerful probe of fundamental excitations in solids, in-
21 cluding those of vibrational or magnetic origins. Neutron scattering from these excitations are
22 characterized by the 4-dimensional (4D) scattering function, $S(\mathbf{Q}, E)$, where \mathbf{Q} is the momentum
23 transfer and E the energy transfer. In recent years the use of highly pixelated detector arrays in
24 conjunction with direct-geometry chopper spectrometer (DGS) instruments¹⁻⁷ has allowed for ef-
25 ficient measurements of single crystal 4D $S(\mathbf{Q}, E)$ functions over large ranges of \mathbf{Q} and E . One
26 single measurement of a single-crystal sample at a DGS instrument captures the sample scattering
27 function $S(\mathbf{Q}, E)$ on a 3-dimensional(3D) manifold in the 4D \mathbf{Q}, E space. Typically, a sample is
28 rotated around a single axis, while maintaining a single wavelength (i.e. monochromatic energy)
29 of incident neutrons, to scan the 4D \mathbf{Q}, E volume. A series of 3D manifolds measured during
30 the scan are then combined into the volumetric 4D dataset, allowing for extracting 2D slices at
31 high-symmetry \mathbf{Q} directions by using software packages such as Mantid⁸, Horace⁹, DAVE¹⁰,
32 Mslice¹¹, and Utsusemi¹². This is done by integrating the measured scattering intensity along
33 two of the four dimensions, yielding a scattering intensity as a function of the remaining two
34 dimensions. Most often this is done to extract dispersion relations of fundamental excitations
35 within crystalline solids by illustrating measured scattering intensity as a function of energy trans-
36 fer along the vertical axis and a single direction in wave-vector transfer along the horizontal axis.
37 These extracted dispersion data can be used to directly compare to model calculations of the ma-
38 terials dynamics in order to constrain or refine parameters in a model (i.e. the Hamiltonian). For
39 magnetic systems, SpinW¹³ is often used to fit spin-wave models to the experimentally obtained
40 dispersion along multiple high-symmetry directions simultaneously. This allows one to obtain ex-
41 change parameters or other energy dependent terms in a model Hamiltonian which can represent
42 the spin dynamics of the system.

43 Quantifying a crystalline material's vibrational or magnetic dispersion is key to understanding
44 the system's dynamics. The accuracy of the measured dispersion (and that of the inferred quan-
45 tities which define the dynamics such as exchange couplings or force constants) obtained from
46 DGS experiments are bound by the instrument resolution. However, a significant number of mea-
47 surements do not take into account instrumental resolution effects beyond the use of an analytical
48 approximation of a single energy and wave-vector resolution of the instrument. DGS instrument
49 resolution for the $S(\mathbf{Q}, E)$ scattering function is four-dimensional, and the effects of the resolu-

tion function is compounded by the slope and the curvature of the dispersion surface, making it cumbersome to accurately model. Given a set of instrument and experimental parameters such as chopper settings and the sample shape, the resolution function for DGS neutron scattering instruments still varies at different (\mathbf{Q}, E) points in the measured dynamical range. This resolution ellipsoid varies considerably across the detector array of the instrument as well as energy transfer. Furthermore, the resolution ellipsoid can have significant tilt that can lead to focusing and defocusing effects in the measured dispersion depending upon the slope of the dispersion relative to the tilt. This can make it difficult to accurately extract a model based upon the measured dispersions.

Recently it was demonstrated¹⁴ that some super-resolution imagery techniques can be adapted to improve energy resolution in a phonon density of states measurement, $g(E)$, based upon neutron scattering techniques. This analysis was performed upon a measurement of the phonon density of states as a function of a single independent variable, energy transfer, which is a routine measurement for direct geometry chopper spectrometers measuring powder samples. In this work we introduce a super-resolution technique to improve the ability of extracting dispersion from inelastic neutron scattering measurements of single crystal samples. We use techniques inspired by image correlation methodologies to improve extraction of information from measurements as a function of two independent variables, energy and wave-vector transfer.

II. METHODS

A. Overview

Dispersion relations are obtained from single crystal measurements at DGS instruments by extracting slices of scattering intensity as a function of energy transfer, E , and wave-vector transfer, \mathbf{Q} , along high-symmetry directions in reciprocal space. These slices are obtained by integrating a portion of the measured reciprocal space along the two orthogonal reciprocal space directions to the direction of interest in the chosen slice. Constant \mathbf{Q} cuts through these 2D slices can then be extracted by integrating a portion of the slices along wave-vector transfer and plotting the resulting scattering intensity as a function of energy transfer. For each constant \mathbf{Q} cut through a single 2D slice, centers of peaks in the energy spectrum are recorded as the excitation energies for this particular \mathbf{Q} value. The energy of these peak centers plotted as a function of \mathbf{Q} are the measured dispersions. An analytic or numerical model of the dispersion can then be directly compared to

79 the experimentally determined dispersion values in order to determine model parameters. This is
 80 often done using non-linear curve fitting algorithms. This methodology of extracting dispersion
 81 parameters based upon peak location does not account for instrumental energy or wave-vector
 82 resolution. Such quantities may shift or skew peak locations and therefore would serve to skew any
 83 model parameters determined from comparison of peak positions to model dispersion. The method
 84 we present here calculates resolution based corrections to the measured dispersion functions.

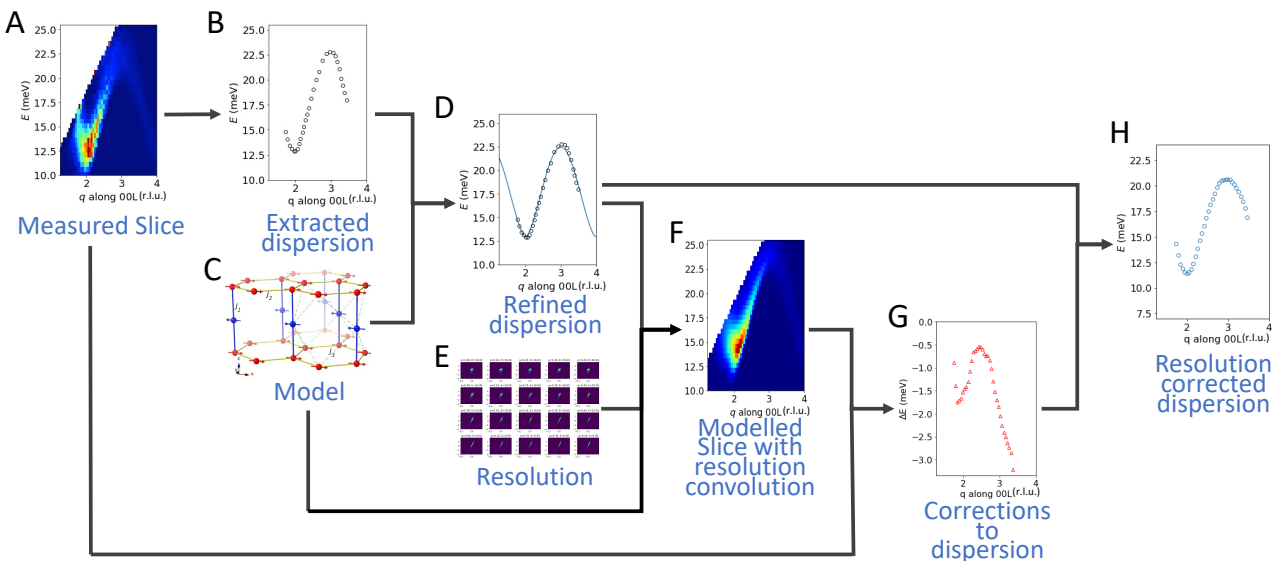


FIG. 1. Super-resolution dispersion workflow. An experimental dispersion (open circles in panel B and D) is first obtained from an experimental slice (panel A). This has been routinely done in single crystal DGS data analysis by finding the peak centers, E_j , of the constant q -cuts, $I(E; q_j)$, to form the dispersion data points $\{(q_j, E_j)\}$. The experimental dispersion is then fit to a dispersion model (an example is shown in panel C) to obtain modelled dispersion (the blue curve in panel D). This preliminary fitting provides a good starting point for the model parameters near the optimal values, and the subsequent steps will make super-resolution corrections. Resolution functions are calculated across the dynamical range of a slice (see panel E). The dispersion model (panel C) with the parameters obtained from fitting done in panel D is convolved with the resolution (panel E) to obtain a modelled slice (panel F). The disparity (panel G) between the modelled slice (F) and the experimental slice (A) is then calculated. Finally, the disparity (G) is used to correct the modelled dispersion (D) and obtain the corrected dispersion (panel H). The units of q are reciprocal lattice units (r.l.u.).

85 Figure 1 shows the steps of this dispersion correction workflow. An experimental slice is first
 86 obtained from data reduction (Figure 1A). A dispersion dataset is then obtained directly from the
 87 experimental slice, $E_{\text{exp};0}(q)$, following the normal steps outlined earlier. This quantity is shown

88 as open symbols in Figure 1B. Those excitations are then fit to a dispersion model (in this case the
 89 spinwave model generated in SpinW) and relevant parameters (in this case exchange parameters)
 90 are obtained (Figure 1A, 1B, 1C, and 1D). The scattering cross section as a function of momentum
 91 transfer and energy transfer, including both the dispersion relation and the scattering amplitude, is
 92 now determined by the excitation model and relevant parameters. The next step is to obtain the
 93 instrument resolution function (Figure 1E). This can be achieved by using analytical calculations
 94 (This is often done for triple axis spectrometers^{15–18}) or Monte Carlo neutron ray tracing simula-
 95 tions. More details can be found in section II B. By convolving the calculated scattering function
 96 with the instrument resolution function we can obtain the modelled slice (Figure 1F). Then we
 97 can compare the modelled slice and the experimental slice and obtain the energy shifts, $\Delta E(q)$
 98 (Figure 1G), required to match the modeled slice to the experimental slice. This step is key to
 99 the super-resolution dispersion determination, and is further explained in section II C. The energy
 100 shifts obtained can then be applied to the model dispersion curve (from first fit to the experimental
 101 data) to obtain corrected dispersion curve (Figure 1H).

$$102 \quad E_{\text{exp};1}(q) = E_{\text{model};0}(q) + \Delta E(q) \quad (1)$$

103 The focus of this work is to demonstrate that measured dispersion relations can be corrected tak-
 104 ing into account resolution effects, but a natural further step is to fit the dispersion model to the
 105 corrected dispersion, $E_{\text{exp};1}(q)$, to obtain the corrected parameters for the Hamiltonian.

106 B. Resolution calculation and convolution

107 The 4D resolution function for a DGS instrument in measurements of single-crystal samples
 108 has been modelled analytically^{19,20}, using covariance matrix to simplify the treatment. It has also
 109 been calculated using Monte Carlo ray-tracing simulations^{21–25}, and was sometimes approximated
 110 using Gaussian functions when it was used in resolution convolution²⁶. However, these corrections
 111 are not often taken into account in 4D DGS data analysis due to the complexity of the resolution
 112 convolution, and the computing resources required for fitting the dispersion model obtained from
 113 a highly pixelated detector array.

114 Incorporating resolution in the single crystal dispersion fitting workflow is difficult because:

- 115 • The resolution is 4D in nature, thus requiring a four-dimensional integration to convolve it
- 116 with a model $S(\mathbf{Q}, E)$.

- 117 • The resolution function varies across the dynamical range, depending on the momentum
118 and energy transfer. For example, as the energy transfer increases the energy resolution
119 broadening decreases for direct geometry chopper spectrometers
- 120 • The resolution ellipsoid can have significant tilt that can lead to focusing and defocusing
121 effects in the measured dispersion depending upon the slope of the dispersion relative to the
122 tilt of the resolution ellipsoid.
- 123 • For some DGS instruments the energy resolution function is asymmetric as a result of the
124 moderation process peculiar to neutron production in spallation neutron sources²⁷.

125 The last point here has very rarely been taken into account previously in single crystal dispersion
126 fitting. Further, to fit the dispersion model incorporating the instrument resolution requires multi-
127 ple evaluation of the dispersion model with varying parameters, as well as resolution convolution
128 with the model for each set of parameters. The number of iterations depends on the optimization
129 algorithm used and how close the initial guess was to the optimal model parameters. Such an
130 optimization procedure can be demanding in both programming and computing resources.

131 The super-resolution procedure outlined in this work is agnostic to the technique of resolution
132 calculation and convolution. In this work we have chosen to use a technique based on the Monte
133 Carlo ray tracing simulation to illustrate the super-resolution methodology.

134 The MCViNE package^{22,28} has been used to compute the resolution function for single crystal
135 measurements at DGS instruments^{22,24,25}. The procedure is reused here to simulate the resolution
136 function (or point-spread function). The simulation starts with a beam simulation that matches
137 experimental conditions such as incident energy and chopper settings. In order to calculate the
138 energy and wave-vector resolution function with MCViNE, we use a virtual sample that has the
139 same geometric shape and lattice parameters of the real sample to scatter neutrons in the vicinity
140 of a particular set of momentum and energy transfer h, k, l, E . In the simulation we also take
141 advantage of the measured UB matrix to orient the virtual sample just like what has been measured
142 during the experiment. The virtual sample is also rotated around the vertical axis to a particular ω
143 angle, similar to what happens in real measurements. The SEQUOIA detector system is simulated
144 according to its specification such as the positions and orientations of all detector packs, the ³He
145 tube radius, length, and its spacing in the detector pack, the pressure of ³He gas in the detector
146 tubes, and the detector pixel height. Only events that arrive at the particular detector pixel and
147 time-of-flight bin corresponding to the nominal h, k, l, E are collected. These detector events are

148 then reduced to $\tilde{h}, \tilde{k}, \tilde{l}$ and \tilde{E} . Those $\tilde{h}, \tilde{k}, \tilde{l}, \tilde{E}$ values center around the nominal h, k, l, E , as expected.
 149 The differences between those $\tilde{h}, \tilde{k}, \tilde{l}, \tilde{E}$ from the nominal h, k, l, E are kept in a list of dh, dk, dl, dE .
 150 The Monte Carlo ray tracing approach captures details of the 4D resolution function including, for
 151 example, the asymmetrical energy dependent line-shape mentioned previously.

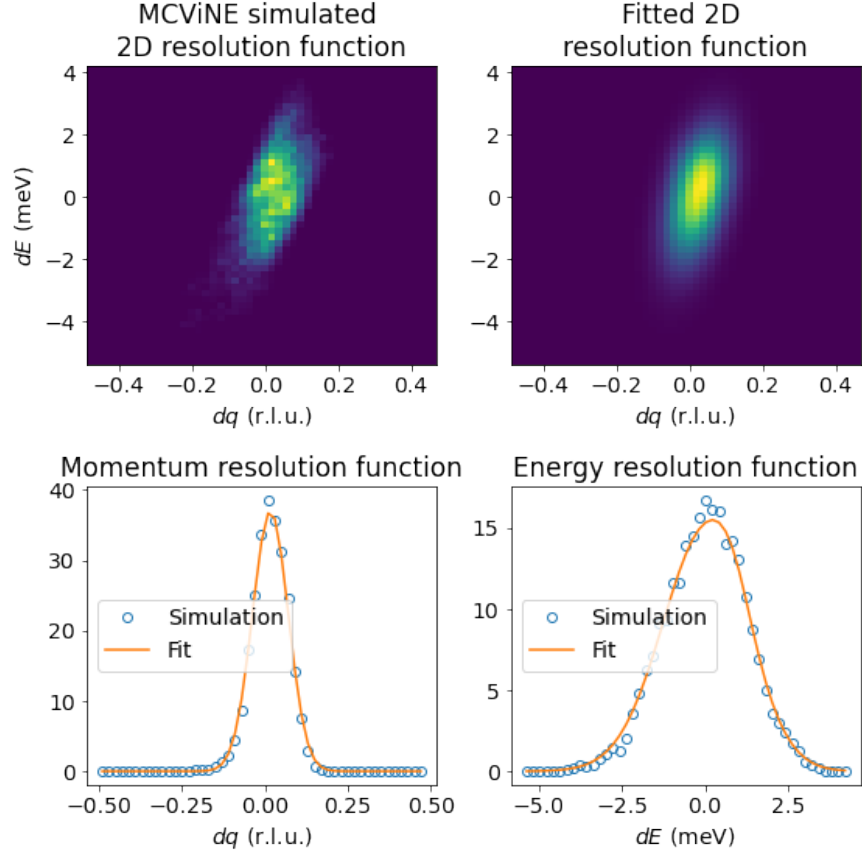


FIG. 2. Example resolution functions for the 00L slice at $q = L = 1.3$, $E = 5.0$. The 2D resolution function $R(q, E)$ is first simulated by using MCViNE, and then fitted to an analytical function.

152 To decrease the complexity of the resolution modeling and convolution, we perform them in
 153 two dimensions along the two axes of a slice. The details of the convolution will be presented later
 154 in this manuscript. We calculate a list of dq from the saved list of dh, dk, dl , where q is along the
 155 high-symmetry Q direction of the slice of interest. The dq, dE events are then histogrammed into
 156 a profile of the point spread function (PSF) for the 2D slice. This procedure is repeated for the
 157 points on a grid on the (q, E) plane. Each PSF at one grid point is fit to a sheared 2D function,
 158 with one axis which is "energy-like" and has an asymmetric shape, and another axis which is
 159 "momentum-like" and modelled as a gaussian. An example of this parameterization is presented

160 in Figure 2. Then an interpolation of the fitted parameters allows us to calculate the PSF function
 161 at any point in the q, E space.

162 Before convolution, the scattering intensities of the dispersion model are first integrated along
 163 the two \mathbf{Q} directions perpendicular to the q direction for the slice of interest. Then the integrated
 164 data is convolved with the 2D resolution function modelled earlier to obtain the convoluted slice.
 165 This convolution method is a good approximation of the full 4D convolution, and an example is
 166 shown in section III B to demonstrate that.

167 C. Correction of dispersions

168 The basic idea here is to compare the two slices, namely the experimental slice (Figure 1A) and
 169 the resolution-convolved modelled slice (Figure 1F), to find the displacements between the disper-
 170 sions in the two images which can then be used to correct the model. Finding displacements (or
 171 disparity) in two images has been a long-standing challenge in image processing. Stereo imaging
 172 techniques that uncover depth information of a scene captured in two images by finding disparity
 173 field between the images have been reviewed multiple times during the last few decades^{29–31}. The
 174 techniques in traditional stereo vision find the disparity field $d(x, y)$ that minimizes the difference
 175 between the left image (image taken by a camera on the left) and the right image (image taken by
 176 a camera on the right) warped by the disparity:

$$177 \quad \arg \min_{d(x,y)} \sum_{x,y} |I_l(x, y) - I_r(x, y - d(x, y))|. \quad (2)$$

178 Used in this formula is the sum of the absolute differences, but often the sum of square differ-
 179 ences, or normalized cross correlation are also used. $I_l(x, y)$ and $I_r(x, y)$ are left and right image
 180 intensities, and $d(x, y)$ is the displacement along y . Local methods for dense disparity calculation
 181 minimize cost functions (Equation 2) for local patches, while global methods^{32,33} and semi-global
 182 methods³⁴ take the smoothness of disparity into account by constraining the disparity $d(x, y)$ us-
 183 ing regularization. Advancements in computing techniques for disparity calculation have been
 184 proven useful in many fields of quantitative research, including remote-sensing and geophysics³⁵.
 185 We aim to reuse the disparity calculation technique to estimate the displacement field between
 186 the experimental slice and the resolution-convolved model slice. In this first demonstrative work
 187 for application of image disparity calculation in the data analysis of neutron scattering measure-
 188 ments, we simplify the problem by limiting the slice to only one visible dispersion; therefore,

189 the displacement field can be simplified to be independent of E , and the minimization problem
 190 becomes

$$191 \quad \arg \min_{\Delta E(q)} \sum_{q,E} |I_{exp}(q, E) - I_{model}(q, E - \Delta E(q))|. \quad (3)$$

192 The simplification of limiting the displacement field to be independent of E makes this optimiza-
 193 tion problem straightforward to program by using a SciPy³⁶ optimizer, for example.

194 III. RESULTS

195 A. The example dataset

196 In this work we illustrate the super-resolution dispersion technique using a synthetic dataset that
 197 resembles a real experimental dataset, for which the full analysis will be reported elsewhere³⁷. In
 198 the experiment, a $\text{Mn}_3\text{Si}_2\text{Te}_6$ single-crystal sample was measured at the SEQUOIA instrument³
 199 with incident energy $E_i = 60\text{meV}$ in the high flux mode, and the sample was rotated at least 180
 200 degrees about the vertical axis, one degree per step, to cover a large volume in the reciprocal
 201 space. Slices along multiple high-symmetry directions show clear dispersions. The dispersions
 202 along those high-symmetry directions were obtained by finding centers of peaks in constant q
 203 cuts. They were fit to a Hamiltonian without on-site anisotropy, but which allows for anisotropic
 204 interactions for each of the exchange interactions to account for the spin-orbit coupling³⁷

$$205 \quad H = J_1 \sum_{\langle i,j \rangle} [S_i^x S_j^x + S_i^y S_j^y + \Delta_1 S_i^z S_j^z] +$$

$$206 \quad J_2 \sum_{\langle i,j \rangle} [S_i^x S_j^x + S_i^y S_j^y + \Delta_2 S_i^z S_j^z] +$$

$$207 \quad J_3 \sum_{\langle i,j \rangle} [S_i^x S_j^x + S_i^y S_j^y + \Delta_3 S_i^z S_j^z]. \quad (4)$$

208 Here, $\{J_i\}$ are exchange coefficients as shown in Figure 3 while $\{\Delta_i\}$ introduce anisotropy.

210 B. Synthetic data

211 First we build a synthetic dataset for which we know the exact model and parameters for the dis-
 212 persion surface. The synthetic dataset is obtained from a virtual neutron experiment performed by
 213 using the MCViNE software. MCViNE contains a scattering kernel that scatters neutrons accord-
 214 ing to a dispersion surface that a user can define by using arbitrary analytical functions^{22,23,28}.

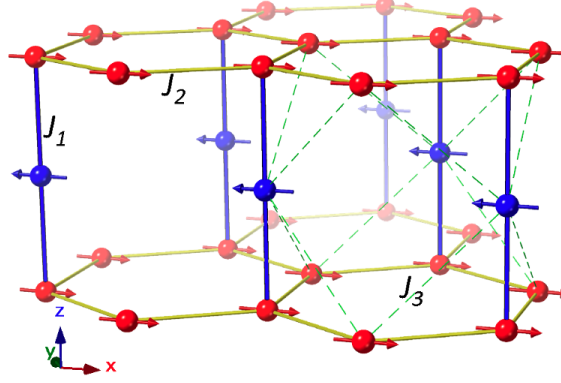


FIG. 3. The magnetic structure of $\text{Mn}_3\text{Si}_2\text{Te}_6$ and the exchange couplings between magnetic sites. The red and blue arrows follow the easy-plane directions of the spins in the ordered phase. The exchange J_1 is between the second nearest neighbor and shown as blue lines between Mn sites. The exchange J_2 is between the first nearest neighbor and shown as yellow lines within the honeycomb layers of the Mn sites. The exchange J_3 is between the third nearest neighbor, and shown as dashed green lines, which are only drawn for one portion of the lattice for clarity of the figure

215 Therefore, an analytical dispersion function similar to the dispersion surface of the spinwave
 216 model defined by Equation 4 was employed. The spin coupling constants used in the spinwave
 217 model in Equation 4 were $J_1 = 1.663\text{meV}$, $J_2 = 0.477\text{meV}$, $J_3 = 0.835\text{meV}$, $\Delta_1 = 0.390$, $\Delta_2 =$
 218 -0.554 , $\Delta_3 = -0.431$. Analytical functions were used to approximate the dispersion and scatter-
 219 ing intensity in the vicinity of the (002) wave-vector, and they were parameterized as

$$220 \quad E(h, k, l) = E_b + E_a \left\{ (1 + 0.61 \sin^2 \pi h)(1 + 0.61 \sin^2 \pi k)(1 + \sin^{1.6} \frac{\pi l}{2}) - 1 \right\} \quad (5)$$

$$221 \quad S(h, k, l) = S0 \frac{1}{1 + \left(\frac{h}{\Gamma_h}\right)^2} \frac{1}{1 + \left(\frac{k}{\Gamma_k}\right)^2} \frac{1}{1 + \left(\frac{l-2}{\Gamma_l}\right)^2} \quad (6)$$

222 where $E_a = 11.6\text{meV}$, $E_b = 9.05\text{meV}$, $S0 = 14.8$, $\Gamma_h = \Gamma_l = 0.38\text{r.l.u.}$, $\Gamma_k = 0.35\text{r.l.u.}$

223 Then we performed a virtual experiment of a sample with this analytical dispersion function and
 224 scattering intensity using MCViNE. The simulation and data reduction consists of the following
 225 steps:

- 226 • Beam simulation. We can reuse the beam simulation performed earlier for the resolution
 227 calculation as it contains all the information regarding the instrument.
- 228 • Sample scattering simulation. The sample has the same geometrical shape as the real sam-
 229 ple, and with the dispersion defined in Equation 6. Simulations with a series of ω rotation

230

angles are performed, matching the real experiment.

231

- Detector simulation. The scattered neutrons are intercepted by the virtual SEQUOIA detector system, and the neutron events detected are saved in NeXus files, one for each ω angle.

232

233

234

- Reduction. The Mantid software⁸ is then used to reduce the NeXus data files in the same way as the real experiment, and corresponding slices are made.

235

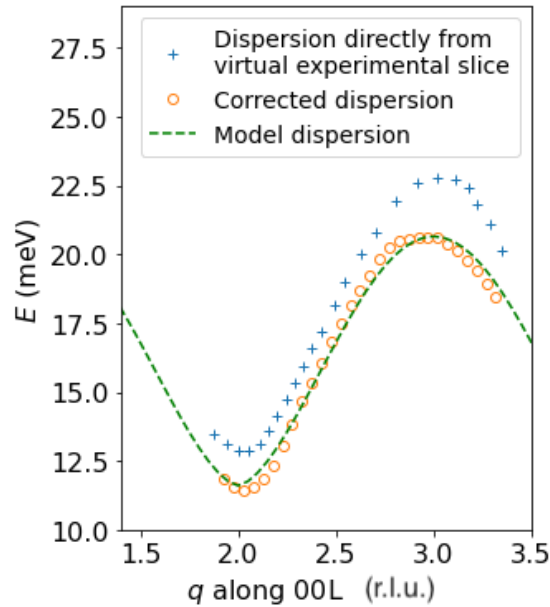


FIG. 4. Dispersion corrections for the virtual experimental data

236

Once we have the virtual experimental data, we perform the super-resolution workflow outlined in Figure 1 upon it. The results are shown in Figure 4. The corrected dispersion shows clear improvement in agreement with the model dispersion curve, compared to the original dispersion obtained directly from the experimental slice. The root-mean-square(RMS) difference between the experimental dispersion data and the model dispersion data was reduced from 1.59 meV to 0.32 meV, showing a nearly 5-fold improvement. It is worth noting that the nominal resolution of the SEQUOIA instrument at $E_i = 60\text{meV}$ for the high-flux mode is $\sim 2\text{meV}$. The fact that one single iteration of our super-resolution workflow can improve the dispersion data accuracy by 5-fold means our method is an efficient way to optimize dispersion model while taking into account the instrument resolution effect.

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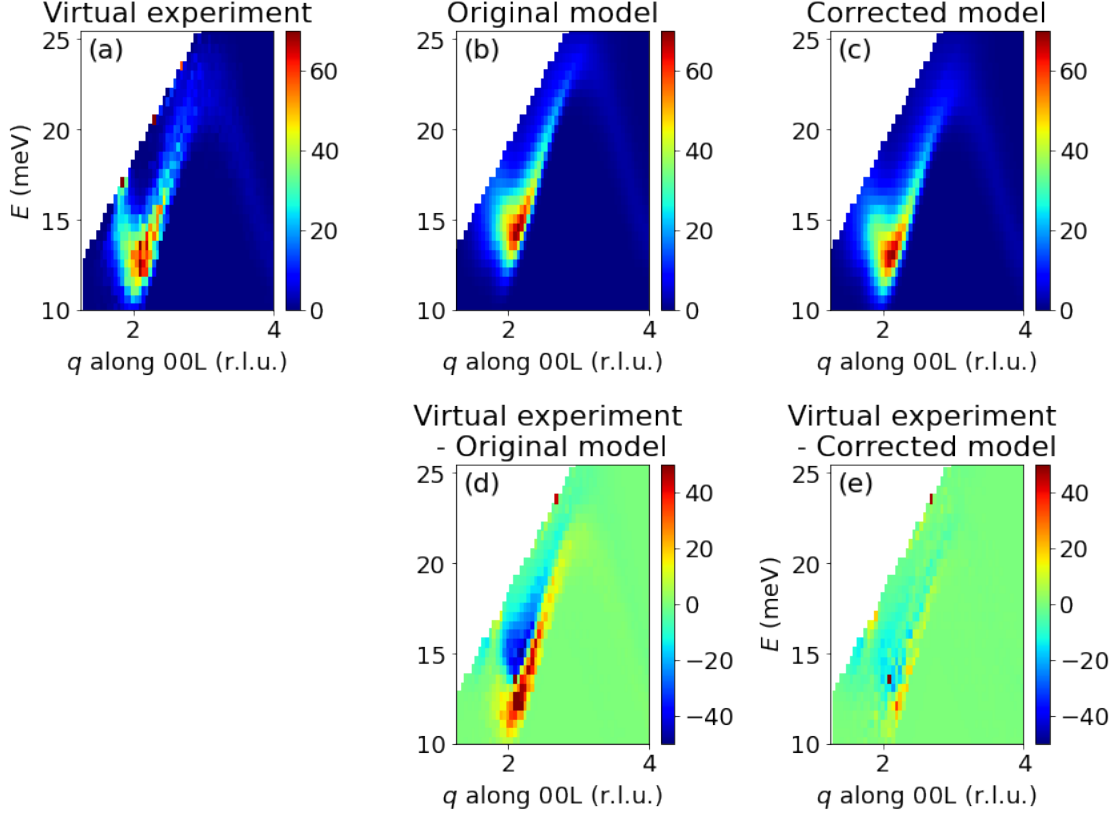


FIG. 5. 00L slices: (a) The 00L slice from the virtual experimental data obtained through the same data reduction procedure as the real experimental data using Mantid. (b) The analytical model using parameters fitted to the dispersion data obtained directly from the virtual experimental data, convolved by instrument resolution using the procedure explained in Section II B. (c) The analytical model using parameters fitted to the corrected dispersion data, convolved by instrument resolution. (d) The residual of subtracting the virtual experimental slice by the original dispersion model convolved with instrument resolution. The root mean square (RMS) of the residual is 10.8. (e) The residual of subtracting the virtual experimental slice by the corrected dispersion model convolved with instrument resolution. The RMS of the residual is reduced to 6.4.

246 Another way to check the improvement of the dispersion data is to observe the improvement of
 247 the fitting parameters in Equation 6. Table I presented the model parameters for the exact model,
 248 the fitted model without resolution correction, and the fitted model with resolution correction.
 249 Without the correction, we obtained $E_a = 12.93\text{meV}$ and $E_b = 9.53\text{meV}$ while fitting the disper-
 250 sion data to Equation 6. Compared to the exact values of $E_a = 11.6\text{meV}$ and $E_b = 9.05\text{meV}$, the
 251 fitted values are off by 1.33meV and 0.48meV , respectively. After correction, the fitting results are

TABLE I. Dispersion model parameters

Model	E_a (meV)	E_b (meV)
Exact	11.6	9.05
Without resolution correction: fit to dispersion data directly obtained from virtual experiment	12.93	9.53
With resolution correction: fit to corrected dispersion data	11.80	8.78

252 $E_a = 11.80$ and $E_b = 8.78$, and the errors are reduced to 0.20meV and 0.27meV.

253 An intuitive illustration of the improvement of the quality of the dispersion model is also pre-
 254 sented in Figure 5. Here, Figure 5(a) is the 00L slice obtained from the virtual experiment data.
 255 Figure 5(b) is the resolution-convolved slice obtained from the dispersion model fitted to the orig-
 256 inal dispersion data from the virtual experiment without correction. It is clear that the dispersion
 257 is shifted upward in comparison to the virtual experimental data in panel (a). Figure 5(c) is the
 258 resolution-convolved slice obtained from the dispersion model fitted to the corrected dispersion
 259 data, and this slice agrees much better with the experimental slice in panel (a). This agreement is
 260 also a validation of our resolution convolution procedure. The better agreement of the corrected
 261 dispersion model with the virtual experimental data is also evident in the residual plots shown in
 262 panel (d) and (e).

263 C. Real experimental data

264 We also applied the super-resolution dispersion workflow on the experimental SEQUOIA
 265 dataset described in section III A. In the previous section for the virtual experimental data, we
 266 apply the super-resolution procedure to one single slice. In comparison, for the real experimental
 267 data, we treat multiple slices along different \mathbf{Q} directions. The first step of the workflow remains
 268 the same; the dispersion data for each slice is first obtained without considering the resolution
 269 effect. Then these dispersion data from multiple slices are fitted to the spin-wave model simulta-
 270 neously to obtain the original set of the model parameters. The fitted model provides dispersion
 271 curves and scattering amplitudes for every slices, and they are convolved with resolution func-
 272 tions to obtained modelled slices. Each modelled slice is then compared to the corresponding
 273 experimental slice to obtain disparity curves, which are used to correct the dispersions. The cor-

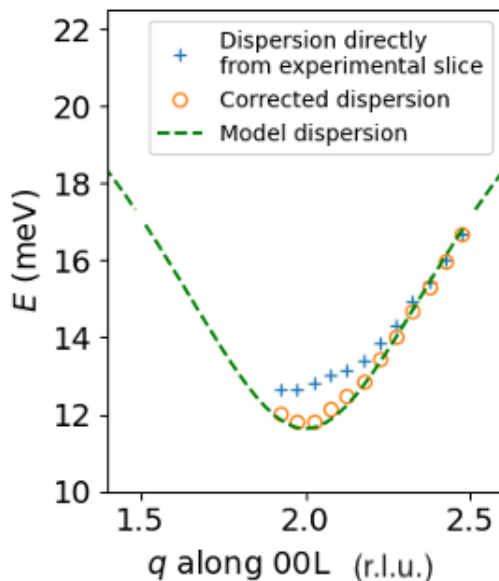


FIG. 6. Dispersion corrections for the real experimental slice along 00L near 002.

274 rectioned dispersions of all interested slices are then fit to the spin-wave model simultaneously again,
 275 yielding a new set of model parameters. One example of the dispersion correction is presented in
 276 Figure 6 for the 00L dispersion. Energy corrections in the order of 1meV are found near 002. The
 277 full dispersion correction data are reported elsewhere³⁷.

278 IV. CONCLUSION

279 A new technique to obtain super-resolution dispersions along high-symmetry \mathbf{Q} directions for
 280 single crystal measurements employing direct geometry neutron spectrometers is developed. This
 281 is done by computing the disparity curve between the resolution-convolved-model slice and the
 282 experimental slice and then applying the disparity to correct the dispersion. Here the resolution-
 283 convolved slice was obtained by convolving the resolution with the scattering intensity of a dis-
 284 persion model that was fit to the experimental dispersions obtained without any consideration of
 285 instrument resolution. The disparity of the slices was obtained by minimizing the difference be-
 286 tween the experimental slice and the modelled slice warped by disparity, subjecting to the total
 287 variation regularization. The technique clearly shows improvements in the determination of dis-
 288 persion and it is computationally faster, since classical methods would have required multiple
 289 iterations of model evaluation and resolution convolution with many more sets of model parame-

290 ters. We show that this method can achieve 5-fold super-resolution w.r.t nominal resolution of the
291 SEQUOIA³⁸ instrument. The demonstration is facilitated by a MCViNE-based virtual experiment,
292 which provides the virtual experimental data and the known target model to check the effectiveness
293 of the super-resolution technique.

294 This super-resolution dispersion technique is limited by the signal-to-noise ratio as other imag-
295 ing techniques. The 2D resolution convolution method used in this work can be updated to use
296 4D resolution convolution to improve the accuracy and the universality of this approach. More
297 sophisticated disparity computation techniques can be adapted to remove the limit of single dis-
298 persion per slice. Finally, many image processing techniques may find various applications in
299 neutron data analysis. Another potential application of the disparity calculation technique is to de-
300 tect super-resolution variations in dispersions w.r.t temperature/pressure under which the sample
301 is measured.

302 This work focuses on the correction of the dispersion relation $E(q)$ between the excitation
303 energy E and its momentum q . It can be envisioned that the super-resolution techniques developed
304 in the previous work for powder DGS data¹⁴ can be extended and combined with techniques
305 developed in this work to reconstruct super-resolution $I(q, E)$ slices, reducing the influence of the
306 instrument broadening, and providing information on the intrinsic line-widths of the excitations,
307 $\Gamma_E(q)$.

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317 **DATA AVAILABILITY**

318 The data that support the findings of this study are available from the corresponding author
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