Lower/Upper Formulae Used in `qe_plot.py`

In the current implementation, the kinematic edge is

$$Q(E,\theta) = \sqrt{\frac{E + 2E_f - 2\cos(2\theta)\sqrt{E_f(E+E_f)}}{\hbar^2/(2m_n)}}, \qquad \frac{\hbar^2}{2m_n} = 2.072\ \text{meV}\ \text{Å}^2. \tag{1}$$

Therefore, with scattering-angle bounds $\theta_{\min}$ and $\theta_{\max}$,

$$Q_{\text{lower}}(E) = Q(E,\theta_{\min}) = \sqrt{\frac{E + 2E_f - 2\cos(2\theta_{\min})\sqrt{E_f(E+E_f)}}{\hbar^2/(2m_n)}}, \tag{2}$$

$$Q_{\text{upper}}(E) = Q(E,\theta_{\max}) = \sqrt{\frac{E + 2E_f - 2\cos(2\theta_{\max})\sqrt{E_f(E+E_f)}}{\hbar^2/(2m_n)}}. \tag{3}$$

The dispersion used in the same script is

$$E_{\text{mag}}(\mathbf{q}) = S\sqrt{A(\mathbf{q})B(\mathbf{q})}, \tag{4}$$

$$A(\mathbf{q}) = J_1(3+2\gamma_1) + 2J_2(-1+\gamma_2)\,, \tag{5}$$

$$B(\mathbf{q}) = J_1(3-\gamma_1) + 2J_2(-1+\gamma_2)\,, \tag{6}$$

$$\gamma_1 = \cos(2\pi q_x) + \cos(2\pi q_y) + \cos\big(2\pi(q_x+q_y)\big), \tag{7}$$

$$\gamma_2 = \cos(\pi q_z). \tag{8}$$

Equivalent coupling products are

$$J_1S, \quad J_2S, \tag{9}$$

because E_{mag} is proportional to S.

Path-coordinate transforms currently used are:

$$\text{(linear path)} \quad |x|_{\text{lower}} = \frac{Q_{\text{lower}}}{|Q_{\text{scale}}|}, \qquad |x|_{\text{upper}} = \frac{Q_{\text{upper}}}{|Q_{\text{scale}}|}, \tag{10}$$

$$\text{(symmetric path)} \quad |x|_{\text{lower}} = \frac{\sqrt{Q_{\text{lower}}^2 - Q_{\text{center}}^2}}{|Q_{\text{scale}}|}, \qquad |x|_{\text{upper}} = \frac{\sqrt{Q_{\text{upper}}^2 - Q_{\text{center}}^2}}{|Q_{\text{scale}}|}. \tag{11}$$

Main parameters used from `list.txt` are:

$$S,\ J_1,\ J_2,\ E_f,\ E_i^{\max},\ \theta_{\min},\ \theta_{\max},\ Q_{110},\ Q_{1\bar{1}0},\ Q_{001}. \tag{12}$$

Numerical values currently used (`code/list.txt`):

$$S = 1.0, \qquad J_1 = 1.80\ \text{meV}, \qquad J_2 = -4.30\ \text{meV}, \tag{13}$$

$$J_1S = 1.80\ \text{meV}, \qquad J_2S = -4.30\ \text{meV}, \qquad E_f = 4.0\ \text{meV}, \tag{14}$$

$$E_i^{\max} = 18.0\ \text{meV}, \qquad \theta_{\min} = 5.0^\circ, \qquad \theta_{\max} = 115.0^\circ, \tag{15}$$

$$Q_{110} = 1.82016\ \text{Å}^{-1}, \qquad Q_{1\bar{1}0} = 1.05087\ \text{Å}^{-1}, \qquad Q_{001} = 0.49986\ \text{Å}^{-1}. \tag{16}$$