4 Supplementary Materials

4.1 Preprocessing

The rods passed into the network are the 16 rods corresponding the region from 00 to 33. q_z ranges from 0 to 6 with Δq_z = 0.025, so our region of reciprocal space is $q_x, q_y \in [0, 3], q_z \in [0, 6]$. This makes each rod of dimension 240, for a total of 3840 points being passed into the network as one flattened array. For the input, due to the many orders of magnitude difference between the Bragg peaks and the in-between fringes, we take the log of the data, where $X_{train} = log(I(\vec{q}))$.

The data is then normalized to mean 0 and standard deviation 1. For the output data, since U_{real} and U_{imag} can have negative values, we apply a transformation where each point is mapped to its z-score relative to all other CTRs simulated in the dataset $\mathcal{D}$. So for a certain point in reciprocal space at (q_x, q_y, q_z), for U_{real}, the transformation looks like: $y^i_{train,real} = (U^i_{real} - \mu_i)/\sigma_i$ where the superscripts and subscripts i correspond to an arbitrary (q_x, q_y, q_z) point, and μ_i and σ_i are calculated using the training dataset $\mathcal{D}$. The process is identical for the imaginary component.

4.2 Training

To train the model, we use a batch size of 32, a learning rate $\alpha = 0.001$, and momentum decay factors $\beta_1 = 0.9, \beta_2 = 0.999$. To optimize the loss function, we use the Adam optimizer[17]. 10^5 CTRs are generated for training on, for which 10% is used for validation. The model is trained for 30 epochs, which is when the validation curve begins to plateau, ensuring the model will not over fit. Each of the two models took $\sim$ 11 hours to train.

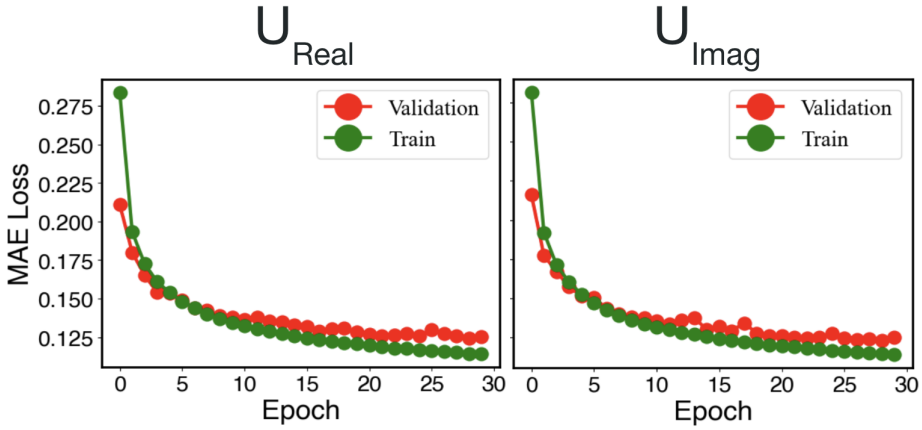

Figure 5: MAE Loss over epochs. The model is trained for 30 epochs, and the best validation error is taken as the final model.

4.3 Field Predictions

For the same electron density map in figure 2, we also plot the corresponding $U(\vec{q})$ prediction for the 00 rod. Note that the predicted field and ground truth field line up quite well, which leads to a good prediction post inverse Fourier transform. We also observe that the random field does not line up with the ground truth field, demonstrating the power of the model to accurately predict the field $U(\vec{q})$.

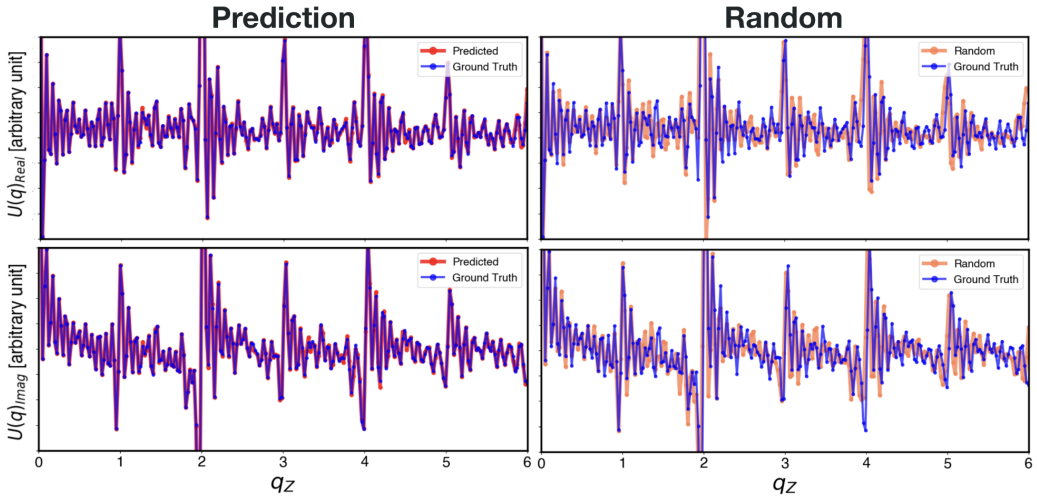

Figure 6: The plots on the left compare the prediction to the ground truth field, $U(\vec{q})$. This field corresponds to the electron density plot in figure 2. For context, on the right we also display the ground truth field against a randomly sampled different ground truth field from the dataset, to emphasize the quality of the prediction. The 00 rod prediction is displayed.