Results of Ray-Tracing the Wavelength Calibration of the Spitzer Infrared Spectrograph

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(Last updated 4 August, 2008)

Abstract

We describe the results of Code-V ray-tracing of the Spitzer Infrared Spectrograph (IRS) to improve the wavelength calibration. For the IRS Short-hi and Long-hi modules, the RMS in $\Delta\lambda$ (observed - calculated) for measured lines has been significantly improved from the purely empirical solution, to 0.125 pixels and 0.091 pixels, respectively. For the Short-lo and Long-lo modules, the RMS is reduced to 0.21 (SL1) and 0.13 (LL1) pixels, respectively. SL2 did not see significant improvement, and the LL2 model produced an RMS larger than the currently used dispersion relation. We therefore propose to adopt the new wavelength calibrations for SH, LH, and LL1.

Motivation and Goals

The wavelength calibration of the IRS modules describes the mapping between spectral order, wavelength, and location along the slit, to pixel coordinates on the detector. For the high-resolution modules, these relations are currently modeled independently for each order by six or seven parameters per order, for a total of 60 or 70 uncoupled parameters. Given the scarcity of strong, unblended lines in some orders, this has made the calibration of these orders somewhat problematic. Similarly, each of the low-resolution modules contains 3 orders, for a total of about 20 parameters describing the wavelength mapping. A physical model such as the Code V optical model couples the orders, so that data in one order constrain the calibration of the other orders, with fewer overall parameters.

In order to develop or refine such a physical model, a request was made to Ball Aerospace by the Spitzer Science Center (SSC) to have the existing Code V IRS model tuned to fit the best on-orbit calibration data. This would have the effect of improving the calibration in all orders, and especially orders in which few calibrator lines have been found. It would also provide physically motivated constraints in the outlying regions of some orders where essentially no constraints exist at present. The work was carried out during the period October 2007 through March 2008. The goal was to make the calibration uncertainty negligible compared to the centroiding error of individual line measurements. The desired accuracy was 0.1 pixels in all illuminated parts of the detector.

Model Inputs

To constrain the Code V model, tables of measured lines were provided to Ball by D. Shupe, formerly of the IRS Instrument Support Team (IST). For each measured line, these tables included the 1) spectral order, 2) the "true" wavelength, corrected for spacecraft motion and radial velocity of the source, 3) the X and Y pixel coordinates of the line on the detector, 4) an estimate of the signal-to-noise ratio of the line, 5) a flag indicating whether the source was compact or extended, and 6) the Reqkey and Expnum of the identifying the observing request and exposure number used for the measurement. In addition, the IRS IST provided Ball with a grid of wavelength, order, and position along the slit, approximately covering the illuminated regions of each detector. These grid values were used by Ball the produce the final mapping of wavelength to pixel location using the tuned Code V model.

Model Outputs

For each IRS module, once the Code V model had been adjusted to fit the appropriate data, the predicted (modeled) X and Y detector locations of each measured line were sent to the IRS IST for review. When the IST determined that the match between the tuned model and the observations was adequate, the X and Y detector locations output by the model for the grid of wavelengths provided by the IST was sent as a final deliverable to SSC. We note that the fidelity of the modeling is primarily limited by the quality and quantity of input data, and less so by the ability to tune the model.

Results

The modeling results were tested by generating pipeline calibration ("wavesamp") files (FITS files relating wavelength to pixel position on the detector) using the Ball-provided grid of wavelengths vs X and Y. Emission lines were measured using both the S17 wavesamp files and the wavesamp files derived using the Code V model. For each wavesamp file, the observed line wavelength was measured and compared with the velocity corrected true wavelength of that line. Observed-predicted line measurements as a function of wavelength for each module are shown in Figures 1 through 4. Lines were measured from some AORs used as inputs for the Code V model, as well as from additional AORs in order to provide a robust test of the new wavelength calibration. The mean offsets and RMSs for all measured lines in each of the IRS modules are summarized and compared with their current S17 values in Table 1.

Table 1: Spectral line measurements vs. model predictions.

Module/Order	S17 Wavesamp		Code V Model-derived Wavesamp	
	Mean Offset (pixels)	RMS (pixels)	Mean Offset (pixels)	RMS (pixels)
SH	-0.019	0.176	0.008	0.125
LH	-0.160	0.185	0.030	0.091
SL1	-0.056	0.223	0.016	0.210
SL2	0.008	0.279	-0.003	0.275
LL1	0.108	0.178	-0.017	0.134
LL2	0.031	0.105	-0.039	0.236

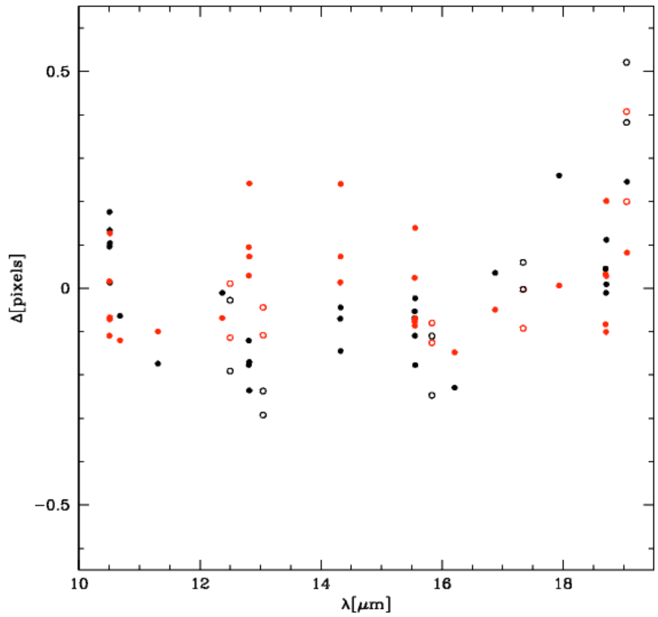

Figure 1. Measured line position using the current, S17 wavesamp (black points) and the Code V model-derived wavesamp (red points) minus true (velocity corrected) line position for the Short-Hi module. Data used as inputs for the Code V model are shown as solid points; open symbols represent data which were not used as Code V inputs. The measured dispersions for the S17 calibration and the Code V modeling results are given in Table 1.

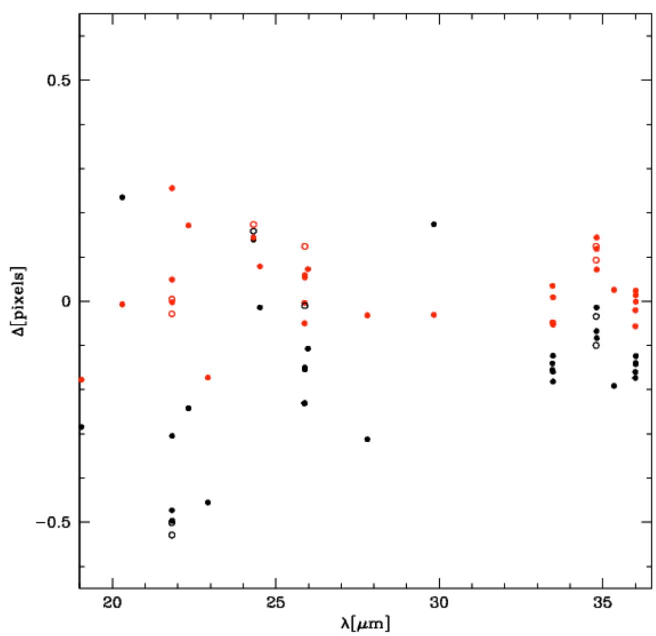

Figure 2. As in Figure 1, but for the Long-Hi model.

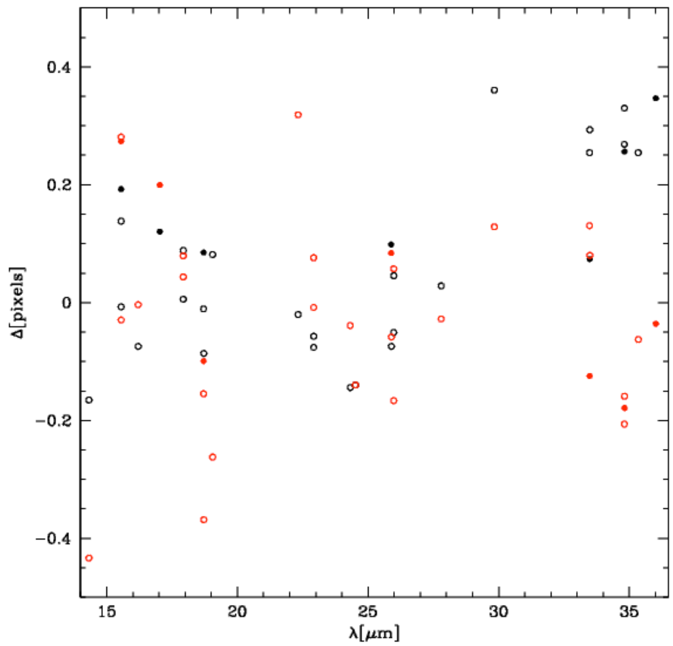

Figure 3. As in Figure 1, but for the Short-Lo model.

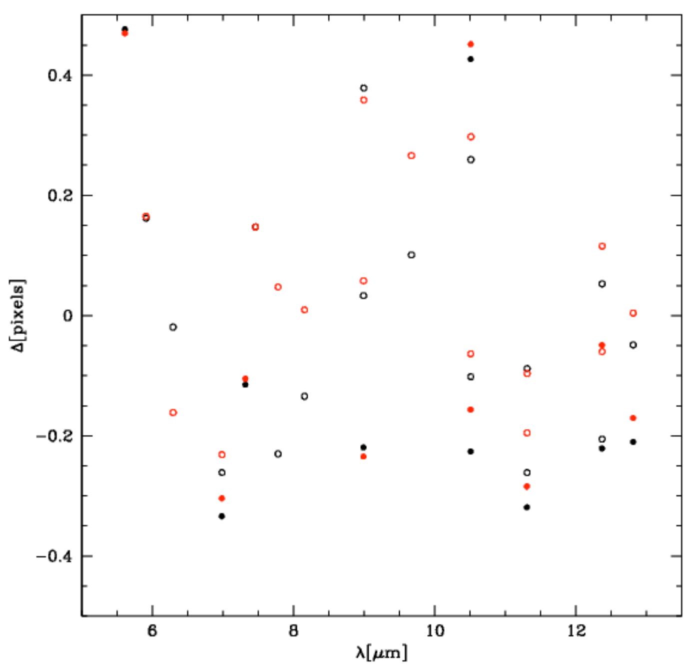

Figure 4. As in Figure 1, but for the Long-Lo model.

The optimized model parameters for the high resolution models are compared with their pre-launch values in Tables 1 and 2. "Spacing" is the grating line spacing in microns per line. "Angle of Incidence" is the incidence angle relative to the grating surface normal. "Clocking" is the orientation of the slit about the grating surface normal with respect to the grating orientation. The parameter adjustments required to match the spectral line measurements are small and appear to be plausible in all cases.

Table 1. Short-Hi Code V Model Parameter Optimization.

Element	Parameter	Nominal	Optimized	Units
Grating 1	Spacing	164.0	163.1	µm
	Angle of Incidence	15.80	15.84	Degrees
	Clocking	0.00	3.93	Degrees
Grating 2	Spacing	340.0	337.1	µm
	Angle of Incidence	29.40	28.89	Degrees
	Clocking	0.00	3.49	Degrees
Focal Surface	X-Translation	0.00	2.28	Millimeters
	Y-Translation	0.00	2.09	Millimeters
	Tilt about X	0.00	1.77	Degrees
	Tilt about Y	0.00	1.38	Degrees
	Clocking	0.00	3.35	Degrees

Table 2. Long-Hi Code V Model Parameter Optimization.

Element	Parameter	Nominal	Optimized	Units
Grating 1	Spacing	164.8	164.4	µm
	Angle of Incidence	16.72	16.80	Degrees
	Clocking	0.00	3.60	Degrees
Grating 2	Spacing	404.3	414.2	µm
	Angle of Incidence	42.06	41.00	Degrees
	Clocking	0.00	3.82	Degrees

Focal Surface	**X-Translation**	**0.00**	**1.94**	**Millimeters**
	Y-Translation	**0.00**	**0.62**	**Millimeters**
	Tilt about X	**0.00**	**0.85**	**Degrees**
	Tilt about Y	**0.00**	**1.72**	**Degrees**
	Clocking	**0.00**	**2.78**	**Degrees**

Conclusions

Using on-orbit spectral line measurements to constrain a Code V optical model of the IRS, we find significant improvements in the resulting wavelength calibration of SH, LH, and LL1. This is particularly important for the high resolution modules, where a relative lack of suitable emission lines has long thwarted our attempts to properly constrain the dispersion relations for individual orders. The goal of 0.1 pixel calibration uncertainty (which is smaller than the individual measurement uncertainties) is largely met or exceeded for SH , LH, and LL1. The new wavelength calibration for these modules will be in place for the S19 reprocessing of IRS data, the results of which will be released in mid-February, 2009.

The results for SL1, SL2, and LL2 are not significantly better than we have been able to achieve empirically, and we propose to continue using the current (July 2008) wavelength calibration until the end of the mission. We note, however, that the refinements of the Code V optical model of the IRS provide us with a functional form for wavelength vs. pixel for all modules. If further improvements to the wavelength calibration are desired in the future, it will now be possible to simply use the model predictions and shift them slightly to match the data, rather than having to conduct Code V modeling all over again.