Q u a n t u m D e s i g n

Application Note 1084-310

ACMS DC Analysis Centering Techniques: Linear vs. Nonlinear Mode

When using the DC extraction method in the ACMS option, one is given a choice of two techniques for tracking the sample center: linear and nonlinear. When making immediate mode measurements, the user must refer to the dialog on the "Configure" tab of the ACMS control center, while when measuring within a sequence this dialog appears in the "Measure" tab of the sequence command.

Before making measurements, the user must center the sample using the "Locate Sample" command. In the ACMS measurement .DAT file, the value "Sample Center(cm)" reflects the sample location that was obtained during the last sample centering operation. The scale for this variable is in motor coordinates, with a value of zero corresponding roughly to an ideal location of the sample.

In contrast to the Sample Center, the "DC Position(cm)" of the sample is determined for each measurement individually. The sample DC Position is found either by using a simple linear Taylor expansion of the extraction data (Linear Mode) or by iteratively shifting the fitting function with respect to the extraction data to obtain the best fit (Nonlinear Mode). These modes are akin to Linear and Iterative regression methods (respectively) used in the MPMS software.

If the DC Position of the sample changes significantly, the linear mode will be less accurate due to the limitations of the approximations used in the analysis (see discussion below). Also, the nonlinear mode will generally be more accurate because it can adjust the center position and get the best fit to the data. However, due to the relative simplicity of the linear mode versus the nonlinear mode which can find "false" minima when fitting noisy data, we recommend using linear mode for small signals ($m < 10^{-3}$ emu).

Based on this, some basic guidelines for making DC extraction measurements in the ACMS are:

1) When possible, measure each data point using both linear and nonlinear modes. When analyzing the data it will often be evident which mode is better, based on the reported "M Std. Dev." values and the guidelines below.

2) Take multiple measurements (at least 3) at each temperature and field so that better statistics are obtained, as "M Std. Dev." is sometimes not representative of the real scatter in the data. Also, drifts in the data will become evident if multiple data points are taken.

3) For large signals ($m > 10^{-3}$ emu), nonlinear mode is best.

4) For small signals, linear mode is required.

5) If measuring moment vs. temperature over any significant range, nonlinear mode is required as the fitting function must be able to shift to truly fit the data instead of just approximating the moment as linear mode does. An alternative to using nonlinear mode is to center the sample ("Locate Sample") frequently as a function of temperature (e.g., every 10 K) and to continue to use linear mode.

Discussion of analysis modes

The calibration data waveform used to fit the extraction data can be described by a function:

$y_{cal} = f(x)$

where y_{cal} is the signal and x is the servo motor position. The measured data will have a dc offset, a different overall amplitude, and some offset Δx in position from the calibration data due to thermal expansion or other effects. This can be described by:

$$y = a + b*f(x+\Delta x) \tag{1}$$

where y is the signal, x is the motor position during the extraction, a is any dc offset, b is the amplitude and Δx is the position offset. Note that the signal y is produced by integrating the induced coilset voltage over position.

LINEAR MODE

This mode uses a linear least squares regression analysis to estimate the value of the position offset Δx and obtain the other unknowns. To obtain the three unknowns, the software performs a least squares fit of the data y to a Taylor expansion of the calibrated signal $f(x)$:

$$y = a + b*f(x) + c*(df(x)/dx) \tag{2}$$

The regression analysis gives a, b and c for the best fit. Once these are obtained, equation (2) is subtracted from equation (1) to obtain:

$$b*[f(x+\Delta x) - f(x)] = c*(df(x)/dx) \tag{3}$$

In the limit that Δx is small (i.e., the sample center has not drifted too far from the original center position), the following general approximation holds:

$$f(x+\Delta x) - f(x) = \Delta x*(df(x)/dx) \tag{4}$$

Comparing equations (3) and (4), we see:

$$\Delta x = c / b \tag{5}$$

The amplitude b is used in the moment calculation and the value of "DC position(cm)" written to the data file is :

$$\text{DC Position(cm)} = \text{Sample Center(cm)} + \Delta x \tag{6}$$

Note that the value of "Sample Center(cm)" is the location of the sample as of the last centering operation and thus does not change if the sample is not recentered.

NONLINEAR MODE

The nonlinear method also uses the Taylor expansion expression (equation (2)) but records the value of the residual of the curve fit (the residual is the quality of the fit, with a value of R = 1 corresponding to perfect correlation). Using equations (3) - (5), a value for Δx is obtained, the measured signal is shifted by Δx, and the curve fit is performed again. This process is repeated iteratively until a minimum in the residual is found. The value of b (in equation (1)) corresponding to the best fit is used to calculate the moment, and "DC Position" is the resulting position of the center of the data.