

## Fourier Transform Limitations

In order to illustrate the difficulties encountered in using Fourier transforms for quantum oscillation data in the cuprates, a comparison can be made with the more favourable situation in the ruthenates.[1] The smallest piece of Fermi surface in  $\text{Sr}_2\text{RuO}_4$ , the alpha pocket, has a frequency of 2.6 kT. Because the  $T_c$  is so low, 1.43 Kelvin, the oscillations are visible at very low fields, and there are about 800 visible oscillations between 3 and 33 Tesla; the larger Fermi pockets have several thousand oscillations in this same range. When Fourier transforming a finite number of oscillations, the resulting frequency spectrum is a convolution of the Fourier transform of the oscillating signal, which is a collection of narrow peaks, with the Fourier transform of the boxcar function (which is the sinc function) corresponding to the upper and lower limits of the data. If the number of oscillations within the box is small, then one gets large side lobes and considerable broadening of each peak in the frequency spectrum. Additionally, because the amplitude of the oscillations is field dependent, the approximately exponential envelope results in a further broadening of the Fourier peaks. In the case of  $\text{Sr}_2\text{RuO}_4$ , Bergemann et al.[2] used Fourier transforms over a window that contains both a large number of oscillations yet a relatively constant amplitude. This fact, coupled with the additional advantage that the oscillation frequencies are well spaced out in frequency space, results in well defined and well separated peaks for each piece of Fermi surface.

For  $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ , the small number of oscillations, the strongly varying background over the field window, and the fact that the frequencies from the two pockets are close together result in broad features in frequency space that overlap each other. Because the Fourier transform gives a complex number, the results are traditionally displayed as the absolute value of this number - a power spectrum. Frequencies that are close together interfere with each other, resulting in relative amplitudes and peak frequencies in Fourier space that do not always reflect the amplitudes and frequencies of the oscillating components in the original data. There are a number of other windows that can be used to apodize the data (other than the boxcar function) in order to decrease the side lobe amplitudes, each having their own tradeoffs (more sidelobes for a narrower central peak, fewer sidelobes for a broader central peak, and mixtures of the two)[3]. None of these address the phase interference of closely spaced frequencies. To quantify the problem, the frequency resolution of a power spectrum

is limited by the number of oscillations measured. With a field range of 30 to 60 Tesla, one is limited to a resolution of  $1/(1/30-1/60) = 60$  Tesla. This is larger than the difference between the average areas of the two pieces of Fermi surface in  $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ . Increasing the upper field range of the measurement to 80 Tesla only increases the resolution to 48 Tesla because the oscillations are periodic in  $1/B$ , so one only gains 2.2 periods of oscillation. If the exact shape of the amplitude envelope and windowing function were known, and there was no problem with background subtraction, the peaks in Fourier space could be fit to a model and the frequencies extracted with much higher precision. However, the exact shape of the background for each surface is not known a priori, so one would still need to do at least some fitting to the original data just to determine the background to be subtracted.

### Genetic Algorithm

Given the difficulties noted above, a direct fit to the raw data is preferable, and can provide highly constrained parameters if the signal to noise ratio is high. In the fits presented in this article, even the simplest model has many parameters and must be fit to the entire data set. A very useful tool for this is a genetic search algorithm inspired by evolution as it occurs in nature, taking a heuristic approach to finding the optimal solution rather than a deterministic one[4]. The problem is finding the best set of parameters for a model given a certain set of data points, and the optimal solution is the set of parameters that gives the smallest least squares value. A gradient based search algorithm such as Newton's method may become stuck in local minima if the parameter "landscape" is very rough, making the fit obtained very sensitive to the initial conditions chosen. The genetic algorithm does not take a user-specified starting point, but rather a range for the parameters in which the solution is thought to lie, and then the algorithm randomly generates a large number of starting points. Local minima can be "escaped" by virtue of the design of the algorithm, and the propensity of the algorithm to search outside of the minimum to which it is converging is a controllable parameter. The algorithm proceeds as follows:

1. A large number ( $N$ ) of initial parameter sets (called  $x_{parent}$ ) are created: about 10 times as many sets as there are parameters. In our case the parameters are the average frequency, the warping size, the Dingle factor, an amplitude factor, a phase factor, and  $g * m_s$  (the spin susceptibility); there are two of each of these sets - one for

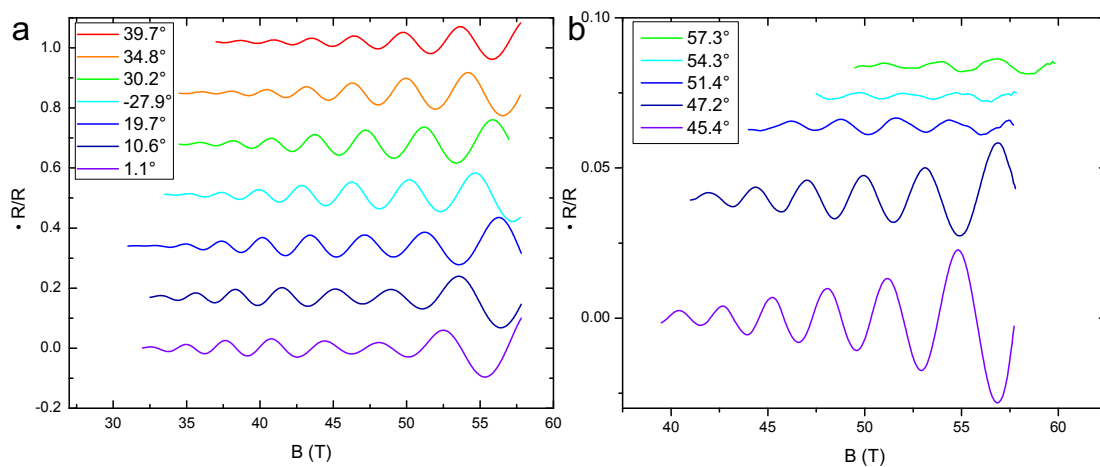
each piece of Fermi surface. Bounds are specified for each parameter in  $x_{parent}$ , and the initial values are randomly generated to lie between those bounds: for example, the average size of the first cylinder could be restricted to lie between 400 and 700 Tesla.

2. A second new parameter set (the “mutated” set) is created by taking three sets at random and creating a new set via  $x_{mut} = x_k + s(x_l - x_m)$ , where  $s$  is a user defined scaling factor. Note that each  $x_i$  is a vector of parameters, so the algebra is performed on each parameter within the vector. If any parameter ends up outside its original specified bounds, then its value is set to the boundary value. This is repeated until there are  $N$  new “mutated” parameter sets.
3. The “crossing” is then performed by taking the  $j^{th}$  set from the parent parameter sets and the  $j^{th}$  set from the mutated parameter sets. Starting with the first parameter (say the average frequency of the first piece of Fermi surface), a new parameter set  $x_{new}$  is created by selecting the first parameter from the original set with probability  $p$ , and from the mutated set with probability  $1 - p$ . This is repeated for each parameter in the set until  $x_{new}$  is completed. This is then repeated for all  $N$  parameter sets.
4. Competition and selection is then effected by computing the sum of the squares of differences between the model with the data points using the parameters from both the  $j^{th}$  set from  $x_{new}$  and the  $j^{th}$  set from  $x_{parent}$  and then keeping the parameter set that has the lowest sum of squares. This is repeated for each of the  $N$  pairs.
5. If the lowest sum of the squares value is less than the tolerance specified, the algorithm terminates, otherwise it returns to step 2.

This algorithm is still capable of becoming stuck in local minima because the initial population is finite, and so was run about a hundred times. Because each run is independent from the others, this can be done in parallel, reducing the computation time. Various adjustments can be made to the algorithm, including (but not limited to): always keeping a few of the best parameter sets from each generation (called “elitism”), penalizing parameter sets that are sitting on the boundary (effectively increasing their least squares value in some artificial way), or even changing the order of some of the steps.

# Parameter Uncertainties

It should be noted that the statistical uncertainties that have been calculated for the fit parameters have not been included in Table 4 because the authors feel that they are much smaller than the uncertainty in the model itself. For example, the largely unwarped cylinder has an average frequency of 526 Tesla has, within the model we used, a statistical uncertainty of  $\pm 0.8$  Tesla. Including higher warping harmonics on the other warped cylinder, adding more Fermi cylinders, accounting for oscillations of the chemical potential itself, including scattering between adjacent Landau levels, and a host of other subtle effects could all change this number by an amount greater than 0.8 Tesla. That being said, we believe that the simplest possible model that reproduces all the features of the data to within the noise of the data is the best starting point.



**FIG. 1: Oscillatory component of the resistance as a function of angle.** **a**, The oscillatory component of the resistance from 1.1 to 39.7 degrees, including a measurement at -27.9 degrees, with the background subtracted. **b**, The oscillatory component from 45.4 to 57.3 degrees. Note that the horizontal axis is just the field  $B$ , not the inverse field scaled by the cosine of the angle.

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