SUPERFIT: a Computer Code to Fit Surface Resistance and Penetration Depth of a Superconductor

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1. Abstract

This note describes a computer code that can be used to perform a mean-square fit of experimental data of surface resistance and penetration depth vs. temperature for a superconductor. As a working example, the results from the measurement of a CEBAF niobium single cell cavity will be analysed with this code.

2. The code

The computer code has been written with Microsoft Visual C++ 6.0[®], which allows the realization of applications in Windows[®] environment, with an easy user interface.

The surface resistance vs. temperature data can be fitted according to a quasi-exponential formula that provides a simplified version of the BCS theory, valid for temperatures lower than half of the superconductor's critical temperature or using the full BCS theory with the code originally written by J. Halbritter [1] and translated in C++ by J. Yan.

The quasi-exponential formula is:

$$R_s(T) = \frac{a_0}{T} \cdot e^{-a_1/T} + a_2 \quad (1)$$

a_2 corresponds to the so-called “residual resistance”, while a_1 corresponds to the ratio between the energy gap at zero Kelvin and the Boltzmann's constant.

The penetration depth vs. temperature data can be fitted according to the Two-Fluid model with Pippard correction for the mean free path [2] or using the full BCS theory. For both surface resistance and penetration depth, the BCS theory calculations are done using a boundary condition of diffuse reflection for the electrons, since it represents a situation closer to the real surface of a superconducting cavity.

The formula that describes the corrected Two-Fluid model is:

$$\lambda(T) = \lambda_L \cdot \sqrt{1 + \frac{\xi}{l}} \cdot \frac{1}{\sqrt{1 - \left(\frac{T}{T_C}\right)^4}} - \lambda(T_0) \quad (2)$$

λ_L is the London penetration depth, l is the mean free path, ξ is the coherence length, T_C is the critical temperature and $\lambda(T_0)$ is an additive constant.

The algorithm that performs the mean square fit of the data is the Levenberg-Malquardt algorithm [3], which can be applied to any non-linear fit. It requires the derivative of the function to be fitted with respect to each parameter and, in case of an analytic function (as the quasi-exponential formula for the surface resistance or the Two-Fluid model for the penetration depth), these derivatives can be calculated analytically but when the data have to be fitted with the BCS theory, they have to be computed numerically:

$$\frac{dy}{da_i}(a_0, a_1, \dots, a_N, T_j) = \frac{y(a_0, a_1, \dots, a_i + h_i, \dots, a_N) - y(a_0, a_1, \dots, a_i, \dots, a_N)}{h_i} \quad i = 0, \dots, N \quad j = 0, \dots, NP$$

for each parameter a_i and temperature value T_j . The increment h has been chosen to be 5% of the parameter's value.

As for any non-linear fit, the initial guess value for the parameters is very important to improve the goodness of fit, since initial values too far from the solution may result in an higher chi-squared or a non-convergent calculation. In general, it's a good idea to run the program with initial values equal to the ones resulted from a first fit of the same data.

There exists a version of the code that runs on a DOS shell and, if compiled with a Linux C++ compiler, can run on a Linux machine as well. The Windows[®] version has been called *WinSuperfit*.

3. Superfit manual and example

This section describes the feature of the Windows version of the program.

When the program is launched, two warning messages appear, regarding a library that has been used in the program and is not registered. Just click the “OK” button after few seconds.

Figure 1: Main program window

The main window shows the four choices to fit surface resistance or penetration depth vs. temperature data. Just click the option you would like to run. Depending on the selected option, a new window appears. On the left there are all the required parameters and a box to be checked if the parameter can be changed during the fit. The default parameters values correspond to niobium.

Figure 2: Window for fitting penetration depth vs. temperature data with BCS theory.

The input data are loaded by pressing the “**Open File**” button and selecting the filename. It has to be an ASCII file (for example a text file) that begins with the number of data points followed by two or three columns of data, the first one being the temperature values in Kelvin, the second one being the surface resistance (in ohm) or penetration depth (in Angstrom) data. The third column is facultative and contains the experimental error for each data point. The input file can be easily created with Excel. The maximum number of data points is 500.

	17	←	Number of points		
Temperature values	{	3.047	1.71053E-07	}	Surface resistance values
		2.976	1.65756E-07		
		2.9	1.44139E-07		
		2.853	1.36024E-07		
		2.804	1.25981E-07		
		2.705	1.03136E-07		
		2.651	1.00073E-07		
		2.497	7.90617E-08		
		2.425	7.49382E-08		
		2.302	5.4242E-08		
		2.204	5.04435E-08		
		2.087	3.85375E-08		
		2.046	3.5888E-08		
		1.987	3.26048E-08		
		1.938	2.91698E-08		
		1.884	2.80778E-08		
1.843	2.66602E-08				

Figure 3: Example of input file

The program then asks if the measurement errors (third column) is included or not in the input file. In case it is, the “Measurement error” field is disabled; otherwise one can set a percentage value for it. The “Calculation accuracy” field refers to the accuracy with which the BCS theory calculations need to be done.

Once the data are loaded, a “guess” value for the parameters has been assigned and it has been decided which parameters to fit for, the “**Fit**” button becomes enabled. By pressing it the mean-square fit algorithm starts. The results are shown on the right side of the window.

Fitting data using the BCS theory takes a lot of time and CPU capability, and the results from each iteration step are shown at the bottom of the window. These include the iteration number, the chi-square, the parameter “alamda”, which is an indication of the variation applied to the fitting parameters, and finally the fitting parameters a_i ($i = 0, 1 \dots 5$) corresponding to the input parameters listed from top to bottom. The calculations can be stopped at any time by pressing the “**Exit**” button and then the “**Quit**” button in the main window.

The screenshot shows the 'WinSuperfit 1.0 - Fit' window. It is divided into several sections:

- Input Parameters:** A list of parameters with input fields and checkboxes for fitting.

Parameter	Value	Fit
Frequency [GHz]	1.5	
Tc [K]	9.442	☐
Gap/kTc	1.85	☐
London pen. depth [Å]	387	☒
Coherence length [Å]	620	☐
Mean free path [Å]	493	☒
Pen. Depth at 0K [Å]	610	☒
Calculation accuracy [%]	1	
Measurement error [%]	5	
- Number of points:** 62
- Fitting Result:** A text area showing the results of the fit.

London Pen. Depth = 386.939 +/- 4.097e+005

Mean free path = 493.278 +/- 1.876e+006

Pen. Depth at 0K = 609.830 +/- 3.924e+000

Chisquare = 89.931
- Fitting:** A large empty text area at the bottom for iteration details.
- Buttons:** 'Open File', 'Fit' (highlighted with a dashed border), 'Plot', 'Save File', and 'Exit'.

Figure 4: Window look after fitting penetration depth vs. temperature data with Two-Fluid model

Once the fitting process is completed, the “**Plot**” button is enabled and allows creating a plot of the input data along with a curve describing the fitted function. The plot function has been done using a graphic library included in the book in ref. [4].

Figure 5: Window that shows input data and fitted function

Pressing the “**Save File**” button, it is possible to save the initial parameters values, the values after the fit with the chi-square, the input data along with the data obtained from the fitted function and finally the experimental errors.

For example, in figure 6 are shown the results from a fit of the variation of penetration depth with temperature on a CEBAF niobium single cell cavity using the Two-Fluid model. The parameters that could be adjusted during the fit had been chosen to be the critical temperature, the mean free path, the London penetration depth and the additive constant.

Result from fitting Penetration Depth vs. T with two-fluid model

Initial parameters:

Critical temperature (a1) [K] = 9.442

London penetration depth (a2) [Å] = 387

Coherence length (a3) [Å] = 620

Mean free path (a4) [Å] = 493

Penetration depth at 0 K (a5) [Å] = 610

chi-squared = 89.9298

a1 = 9.44219 +/- 0.00553882

a2 = 386.993 +/- 400186

a4 = 493.032 +/- 1.83054e+006

a5 = 609.997 +/- 6.25004

T [K]	Lambda [Å]	Lambda fit [Å]	stdev [Å]
5.205	0.321	0.323	0.016
5.510	11.543	8.423	0.577

T [K]	Lambda [A]	Lambda fit [A]	stdev [A]
5.830	24.048	18.962	1.202
6.120	33.988	30.747	1.699
6.375	41.683	43.284	2.084
6.605	48.096	56.738	2.405
6.850	67.013	73.834	3.351
6.900	72.785	77.733	3.639
6.950	77.274	81.789	3.864
7.000	83.686	86.007	4.184
7.050	88.496	90.398	4.425
7.105	92.023	95.438	4.601
7.160	96.512	100.710	4.826
7.210	103.245	105.718	5.162
7.265	108.055	111.476	5.403
7.310	111.582	116.393	5.579
7.370	116.392	123.257	5.820
7.420	121.522	129.263	6.076
7.475	130.820	136.190	6.541
7.525	140.760	142.799	7.038
7.580	150.700	150.437	7.535
7.640	158.395	159.241	7.920
7.695	163.846	167.779	8.192
7.750	176.030	176.804	8.802
7.805	190.138	186.355	9.507
7.860	202.322	196.477	10.116
7.910	208.735	206.220	10.437
7.965	219.316	217.584	10.966
8.025	232.142	230.830	11.607
8.085	249.777	245.056	12.489
8.145	265.809	260.376	13.290
8.195	283.444	274.072	14.172
8.250	298.514	290.228	14.926
8.305	314.866	307.657	15.743
8.365	331.539	328.315	16.577
8.425	353.663	350.933	17.683
8.475	376.749	371.496	18.837
8.530	400.797	396.186	20.040
8.585	430.296	423.380	21.515
8.645	467.490	456.405	23.374
8.695	502.439	487.090	25.122
8.755	546.046	528.483	27.302
8.805	589.653	567.573	29.483
8.860	639.672	616.520	31.984
8.905	695.463	662.262	34.773
8.960	770.813	726.961	38.541
9.020	854.179	811.964	42.709
9.085	970.250	927.929	48.512
9.150	1125.759	1081.605	56.288
9.220	1329.044	1319.053	66.452
9.220	1348.603	1319.053	67.430
9.225	1370.085	1340.354	68.504

T [K]	Lambda [A]	Lambda fit [A]	stdev [A]
9.235	1388.041	1385.275	69.402
9.240	1409.844	1408.991	70.492
9.245	1429.403	1433.613	71.470
9.250	1447.038	1459.201	72.352
9.255	1466.277	1485.819	73.314
9.260	1489.363	1513.536	74.468
9.265	1511.166	1542.432	75.558
9.270	1530.084	1572.589	76.504
9.275	1550.284	1604.103	77.514
9.280	1570.484	1637.078	78.524

Figure 6: Example of fit of penetration depth vs. temperature.

It can be seen that the estimated error of London penetration depth and mean free path are quite large. This is due to the nature of formula (2), and a more realistic error can be obtained by fitting separately for the two parameters.

The computer code can be requested by sending an e-mail to gciovati@jlab.org.

4. Acknowledgements

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5. References

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