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Considerations Relating to Type 1 and Type 3 Non-uniqueness in SPRT Interpolations of the ITS-90

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Abstract It is well known that different allowed interpolations using a given standard platinum resistance thermometer (SPRT) in overlapping subranges of the ITS-90 do not lead to identical results. This is termed Type 1 non-uniqueness, or subrange inconsistency (SRI), and it arises because of small incompatibilities in the SPRT characteristic $W(T_{90})$ with respect to the ITS-90 reference function $W_r(T_{90})$, such that the alternative low-order interpolations, fitted to the deviations $W(T_{90}) - W_r(T_{90})$ at different sets of fixed points, are not in general identical. To some extent SRI may be 'scale-intrinsic,' i.e., caused by incompatibilities between the resistance ratios, $W_r(T_{90})$, specified at the fixed points of the ITS-90, and hence the same for all SPRTs. However, it has been found that the SRI varies strongly between different SPRTs, and that variability of $W(T_{90})$ is much the dominant cause. This raises the question of how SRI is linked to Type 3 non-uniqueness between SPRTs in each separate subrange, which is *entirely* due to differences in SPRT characteristics. This paper explores the connection between them and concludes that they are of similar magnitude and consequently, being different manifestations of the same effects, it is argued that non-uniqueness should be covered by a single component of uncertainty. Following the stated rationale of the ITS-90, it is further suggested that this uncertainty should be estimated only within each subrange, i.e., that shorter subranges should not be deemed subject to potential effects caused by out-of-range data.

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1 Introduction

The ‘non-uniqueness’ of the ITS-90 is the term given to the variability of values of T_{90} which may be obtained even if the procedures of the ITS-90 are followed as specified and the experiments are carried out perfectly. Three kinds of non-uniqueness have been identified [1], of which two are relevant to the use of standard platinum resistance thermometers, SPRTs, and are discussed here. Type 1 non-uniqueness (also known as subrange inconsistency, SRI) arises because *for a given SPRT* the ITS-90 allows alternative interpolations in overlapping subranges, and these are not in general identical. Type 3 non-uniqueness occurs because *in a given subrange* different SPRTs which qualify for use give slightly different interpolations.

In the ITS-90 interpolations the differences $W(T_{90}) - W_r(T_{90})$ between SPRT resistance ratios, $W(T_{90}) \equiv R(T_{90})/R(273.16\text{ K})$ or simply W, and values of the reference resistance ratios, $W_r(T_{90})$, or simply W_r, are expressed as polynomial ‘deviation’ functions of W. These functions are derived using values of W measured at the fixed points and the corresponding specified W_r values. The W_r values were chosen so that, as far as could be ascertained, the differences between the various subranges (the SRI) would be small: any incompatibility between the W_r values, being the same for all SPRTs, would result in ‘scale-intrinsic’ SRI. Several studies have shown that the mean SRI (which is conveniently taken as the scale-intrinsic component) is small, but that the SRI of individual SPRTs is significantly dispersed about this mean.

Type 3 non-uniqueness (here abbreviated to NU3) arises entirely because the characteristics of SPRTs are not completely accommodated in the ITS-90 interpolations. As a result different SPRTs give slightly different values at temperatures between the fixed points in a given subrange. If SPRTs interpolate differently in one subrange, we must expect them do so in any other subrange, and by amounts that are in general different, because different sets of fixed points and polynomials are used. The SPRT dependence of both the SRI between two subranges and the NU3 within the two subranges implies that there must be a link between them.

This paper discusses these questions mainly with reference to the subranges from the triple point of water (TPW) to the freezing points of zinc and aluminum. It draws conclusions about the relative magnitudes of the scale-intrinsic and SPRT-dependent components of SRI, and the uncertainty of the SRI determination. It then examines the connection between SRI and NU3 more fully than has been done before, by developing a simple argument to show how SRI and NU3 are linked. The implications for estimating the non-uniqueness uncertainties in the realization of the ITS-90 using SPRTs are explored, and a proposal is made for treating SRI (and non-uniqueness generally) without accepting additional uncertainty due to effects which may arise from out-of-range measurements.

2 Subrange Inconsistencies in SPRT Interpolations

SRI in SPRTs has been widely studied [2–9] because it can easily be calculated given data at all of the fixed points specified in both the subranges concerned. Studies were undertaken in the years leading up to the adoption of the ITS-90, and several publications followed soon afterward [2–4]. Further studies have been published more recently [5–8], and we here refer to some data collated at NPL [9]. See "Appendix 1" for more details.

In contrast to this, the determination of Type 3 non-uniqueness between SPRTs is difficult: in order to calculate the differences in the interpolated temperatures we need to know the values of $W(\mathrm{A})$ and $W(\mathrm{B})$, for SPRTs A and B, that correspond to the same temperature. Therefore, NU3 must be determined by making direct or indirect isothermal comparisons between the SPRTs. Good comparison data are available below the triple point of water, TPW, for sets of capsule-type SPRTs which can be precisely compared in cryostats [10, 11]. However, comparisons of long-stem SPRTs as used above the TPW are not easy and the best NU3 data for them come from indirect comparisons using measurements at additional fixed points such as the gallium, indium or cadmium points [12]. In view of the limited amount of data available, it is useful to investigate the SPRT dependence of SRI to see if it can provide indirect evidence of the magnitude of the SPRT-dependent NU3.

The most important SRI is that between the subranges from the TPW to the aluminum point and to the zinc point, here denoted SRI(Al:Zn), and we now consider this case.

The analysis of SRI(Al:Zn) by Zhiru Kang et al. [5] showed that it can be written

$$\mathrm{SRI}\,(\mathrm{Al{:}Zn}) = (W-1)\,(W-W_{\mathrm{Sn}})\,(W-W_{\mathrm{Zn}})\,c \tag{1}$$

where W_{Sn} and W_{Zn} are the measured resistance ratios at the tin and zinc points, respectively. Equation 1 has the necessary zeros at the common fixed points, and a proportionality with the c-coefficient of the subrange to the aluminum point (forcing zero SRI for the case of a purely quadratic deviation). Thus, SRI(Al:Zn) is scaled by c, and there are analogous equations which relate SRI to the coefficients of the ITS-90 deviation functions in other pairs of subranges [6].

Figure 1 shows SRI(Al:Zn) for a large number of SPRTs which have been calibrated at NPL since 1990 [9]. It has the form expected from Eq. (1), with extrema of − 1.3 mK and + 1.2 mK at about 93 °C (corresponding to c-values in the range $-2.1 \cdot 10^{-5}$ to $+2.0 \cdot 10^{-5}$). Superimposed on this is a bold line showing the mean SRI and dotted lines showing the standard deviation of the dispersion of the SRI for the SPRTs in this group (± 0.41 mK). Other studies [5–8] show similar results.

Three important conclusions follow. The first is that the scale-intrinsic component of SRI(Al:Zn) is quite small, ∼ ± 0.2 mK. A scale deficiency, being the same for all SPRTs, would lead to a bias in the SRI: ideally the mean value for a 'representative' group of SPRTs should be zero. In practice no group can be truly representative, but the estimate of ± ∼0.2 mK encompasses the mean values of this and other groups studied (see "Appendix 1"). We note in passing that the NPL group showed some

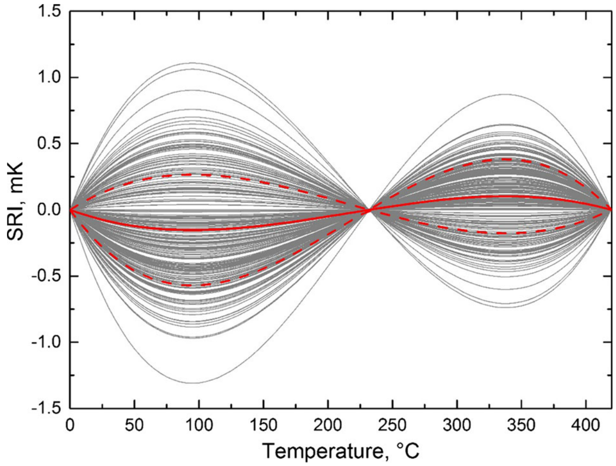

Fig. 1 SRI(Al:Zn) determined at NPL [9] from data for a total of 159 SPRTs (and 62 repeat calibrations). The solid red line shows the mean SRI of the set, and the dashed red lines show one standard deviation in the dispersion of values about the mean (Color figure online)

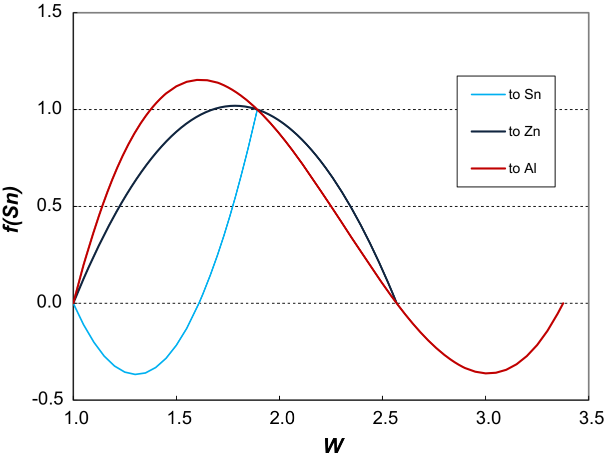

Fig. 2 Uncertainty propagation function $f(\mathrm{Sn})$ in ITS-90 subranges to the tin, zinc and aluminum points. Its effect on the SRI(Al:Zn) is much attenuated because of the similarity of the propagation of $u(W_{\mathrm{Sn}})$ in the two subranges (Color figure online)

dependence on the manufacture of the SPRTs, which is responsible for the slightly negative mean value at 93 °C.

The second conclusion is that the uncertainty in determining SRI(Al:Zn) is quite small. Zhiru Kang et al. [5] presented an analysis which showed that $u(\mathrm{SRI(Al{:}Zn)})$ is much attenuated compared with the uncertainties of the fixed point data, $u(W_{\mathrm{Sn}})$, $u(W_{\mathrm{Zn}})$, and $u(W_{\mathrm{Al}})$. This can be represented graphically by plotting the uncertainty propagation of each fixed point in the various subranges, using the Lagrange functions given in Section 6.2 and Appendix 1 of [12]. Thus, Fig. 2 plots the propagation functions f_{Sn} for the subranges from TPW to the Sn, Zn and Al points, where it can be seen that a given error in W_{Sn} produces similar effects in the subranges to the Zn and Al points, and hence very little SRI between them, at most only $\sim$25 % of $u(W_{\mathrm{Sn}})$. The maximum SRI due to errors at the zinc point is also only $\sim$25 % of $u(W_{\mathrm{Zn}})$. The uncertainty propagated by $u(W_{\mathrm{Al}})$ in the subrange to FP(Al) is always less than 0.1 $u(W_{\mathrm{Al}})$ below the zinc point.

This conclusion applies to other cases of SRI where the propagation functions are similar, but note that it does not apply with respect to the subrange to the Sn point, in which $u(W_{\mathrm{Sn}})$ propagates very differently, see Fig. 2, due to the inclusion of the indium point.

Thus, SRI(Al:Zn) for any SPRT can be calculated quite accurately; for example, if the standard uncertainties $u(W_{\mathrm{Sn}})$= $u(W_{\mathrm{Zn}})$ = 0.5 mK and $u(W_{\mathrm{Al}})$ = 1.0 mK, the standard uncertainty in the SRI at 93 °C is only $\sim$0.19 mK.

This leads to a third conclusion: the dominant SPRT dependence of SRI(Al:Zn) in Fig. 1 is real, not due to propagation of experimental error. As SRI and NU3 both originate, to a large extent, from the variability of SPRT characteristics, it is important to look for the link between SRI, which can easily be determined, and NU3, which cannot.

To do this, the following simple analysis applies.

The SRI in subranges 1 and 2, I_{12}, is the difference between interpolated temperatures T_1 and T_2. For SPRT A this can be written as

$$I_{12}(\mathrm{A}) = T_1(\mathrm{A}) - T_2(\mathrm{A}).$$

Similarly for SPRT B we have

$$I_{12}(\mathrm{B}) = T_1(\mathrm{B}) - T_2(\mathrm{B}).$$

The NU3 between SPRTs A and B in subrange 1 can be written

$$N_1(\mathrm{A,B}) = T_1(\mathrm{A}) - T_1(\mathrm{B}),$$

and similarly for subrange 2 we have

$$N_2(\mathrm{A,B}) = T_2(\mathrm{A}) - T_2(\mathrm{B}).$$

Hence, by subtraction it follows that

$$N_1(\mathrm{A,B}) - N_2(\mathrm{A,B}) = I_{12}(\mathrm{A}) - I_{12}(\mathrm{B}) \tag{2}$$

at any point common to both subranges. The analysis can be extended to groups of SPRTs, in which case N_1, N_2 and I_{12} are characterized by distributions of NU3 and SRI for SPRTs A, B,.. (as in Fig. 1).

3 Implications for Non-uniqueness Uncertainties in SPRT Calibrations

Given that SRI can be directly determined from the measurements at the fixed points, the link in Eq. (2) should be useful in estimating the likely magnitude of NU3 in the ITS-90, which is difficult to measure. However, the link is only between *differences* in NU3 and SRI, and the magnitudes of $N_1(1,2)$ and $N_2(1,2)$ could in principle be much larger than the differences. If we take two SPRTs which lie on the positive and negative standard deviation curves of the SRI in Fig. 1 we have $I_{12}(1) - I_{12}(2) \sim 0.82$ mK at 93 °C, and therefore $N_1(1,2) - N_2(1,2) \sim 0.82$ mK. The values of $N_1(1,2)$ and $N_2(1,2)$ are unknown, but suppose $N_2(1,2) \sim 0$ mK, then $N_1(1,2) \sim 0.82$ mK. This is already large compared with the experimental estimates of NU3 in this range, ~ 0.5 mK (see Figure 10 of [12]), suggesting that estimates of NU3 of these magnitudes in reality duplicate the uncertainty components due to SRI. It should also be remembered that NU3 is inherently a *dispersion* of values about some chosen reference, often the mean value, so a skewed distribution, such as 0 mK to 0.82 mK, is not meaningful: the NU3 would be expressed as ± 0.41 mK.

These conclusions are necessarily speculative, because the analysis is based on interpolations for different SPRTs in the two subranges, which in turn are based entirely on data at the fixed points. Whereas SRI(Al:Zn) is *exactly* the difference between two such interpolations, dependent on the value of the c-coefficient, NU3 arises from the real variabilities in SPRT characteristic, not that between the approximate interpolations of the ITS-90. Thus, NU3 cannot be derived from fixed point calibration data alone: it has the form of Eq. 1 but the constant c is replaced by an unknown function $g(W)$ [8,12]. In practice, resistance anomalies due to impurities or differences in atomic structure or states of anneal, etc., which are responsible for NU3, occur over broad ranges of temperature, so $g(W)$ is a slowly varying function. Even at low temperatures, where the differences between SPRT characteristics are more significant relative to the values of W, the estimated standard deviations of NU3 are quite small (< 0.15 mK). Much of the structure in NU3 data [10,12] superimposed on the oscillatory form of Eq. 1 can be attributed to experimental imprecision, not real effects.

4 How Should Non-uniqueness be Treated?

SRI is a consequence of the decision, in formulating the ITS-90, to allow overlapping interpolations starting from the triple point of water and extending to progressively higher (or lower) fixed points (because for various reasons it is not desirable to define extensions piecewise from one point to the next). This was done to facilitate realizations over only as wide a range as is needed, because SPRT calibrations in shorter subranges are less demanding and more economical, and they are potentially more precise. While the ITS-90 asserts that ‘these differing definitions have equal status’ [13], they do not have equal uncertainty. It was left to the Supplementary Information to explain the rationale in more detail, where it is written (in the 1990 version [14], Page 8) that ‘one of the guiding principles in setting up the ITS-90 was that it should allow the user as much choice in its realization as was compatible with an accurate and reproducible scale’.

Thus, for example, the melting point of gallium was introduced to ‘offer the simplest possible way of achieving the highest accuracy thermometry in the room temperature range’ [14]. It was clearly intended that the realization and its uncertainty should be considered without reference to the possible differences with respect to overlapping realizations which extend to higher temperatures, the values of $W(\mathrm{In})$, $W(\mathrm{Sn})$, etc, being of no relevance.

In the same way, in a realization up to the tin point, based on values for $W(\mathrm{In})$ and $W(\mathrm{Sn})$, the hypothetical values of $W(\mathrm{Zn})$, $W(\mathrm{Al})$ are not relevant, and similarly a realization up to the zinc point should not be contingent on whatever value or uncertainty might apply if $W(\mathrm{Al})$ is measured. Thus, in this view SRI(Al:Zn) affects only the subrange to the aluminum point, and not the subrange to the zinc point.

This leads us to propose a less rigid treatment of SRI and NU3 than that adopted in [12]. We suggest that the subrange to the gallium point is treated as having no SRI and is only subject to Type 3 non-uniqueness (which in practice may be unmeasurably small). If measurements are needed beyond 30 °C, the realization must extend at least to the indium point, and the subrange to the indium point incurs the SRI between the two subranges, to the extent that the a-coefficients are different, as well as a somewhat larger Type 3 non-uniqueness. To proceed beyond the indium point requires measurement at the tin point, which incurs SRI with respect to the gallium and indium subranges, and again larger NU3. So the process continues, up to the aluminum point, but at no stage does a higher, out-of-range, measurement influence the lower subranges.

We believe that this is a more ‘consumer-centric’ view which allows users with demanding requirements over limited ranges, as in electrical and dimensional metrology and oceanography, to minimize their uncertainties without extraneous components arising from wider subranges. Where two SPRTs with calibrations in different subranges are used or compared, the non-uniqueness uncertainty of each subrange is different and need only be applied to that subrange. This contrasts with the ‘supplier-’ or ‘NMI-centric’ treatment in which the full range ITS-90 has some preferred status and its non-uniqueness has a bearing on all the lower subranges.

5 Conclusions

Using published and new experimental data for the inconsistency of SPRT interpolations from the triple point of water to the zinc and aluminum points in the ITS-90, it is concluded that the major factor determining the magnitude of SRI(Al:Zn) is the variability of SPRT characteristics: scale-intrinsic effects are comparatively small, as are the typical experimental uncertainties in its determination. This SPRT dependence implies that SRI and Type 3 non-uniqueness are to a large extent different manifestations of the same effects, and a link between them has been investigated which suggests that they are of comparable magnitudes.

Therefore, it is proposed that estimates for uncertainties due to non-uniqueness should not include components from both sources unless the correlations are properly taken into account. Following the original rationale for introducing subranges, it is suggested that shorter subranges should not be burdened by effects due to out-of-range data (which often do not even exist), and that SRI in a given range should be considered only with respect to subranges which are contained within that range, but not outside it. This does not imply suppressing any uncertainty, but only applying it where it belongs.

To date, SRI has not been extensively studied between all pairs of subranges, and it is desirable that it should be, in order to derive accepted values for their typical magnitudes. These can be adopted for inclusion in uncertainty estimates where the SRI has not been determined, i.e., where not all the fixed points within the subrange have been measured.

It is also desirable that NU3 is measured in other subranges, through comparisons of SPRTs as well as at redundant fixed points. This will not be easy, and it is suggested that measured values are checked against estimates from SRI data, using the link described in this paper.

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Appendix 1. Further Discussion of Results for SRI(Al:Zn)

The results of recent studies into SRI(Al:Zn) are summarized in Table 1. For each source the number of SPRTs studied is given with, in parentheses, a smaller number after any outliers have been removed. The mean and standard deviation of the SRI at 93 °C are then given for the full and the reduced samples of SPRTs.

The elimination of outliers needs careful consideration: in principle it is possible that an SPRT could produce results which lie away from the rest (though one wonders what this might mean for the composition or condition of the platinum wire). On the other hand, SPRTs are not perfectly stable and the conclusions would be corrupted if bad data or cases of instability are included. In fact four of the outliers in Zhiru et al. [5] were documented in the original publication [4] as having been unstable. In other cases, it may be difficult or impossible to identify the causes of discrepant results. It suffices to say that in Table 1 the standard deviations are significantly reduced by the

Table 1 Summary of the results of five studies of SRI(Al:Zn); see the text for explanations

Source	Sample	All data		Excluding outliers	
		Mean / mK	SD / mK	Mean/mK	SD/ mK
Zhiru Kang et al. [5]	65 (58)	– 0.53	1.79	0.06	0.32
Zhiru Kang et al. [6]*	21 (20)	– 0.03	0.93	– 0.22	0.36
Sun et al. [7]	60 (59)	0.20	0.37	0.23	0.29
White & Strouse [8]	60 (60)	0.12	0.48	0.12	0.48
NPL (8 suppliers) [9]	159 (158)	– 0.14	0.52	– 0.12	0.41
NPL (excl. most Tinsleys)	61 (60)	0.05	0.68	0.12	0.40

*The authors are grateful to Dr Zhiru Kang for sending the data for SRI(Al:Zn) for this group of SPRTs, which were not published in [6] elimination of the outliers, all which are more than three standard deviations away from the mean of the rest of the group.

An interesting feature of Table 1 is that the large NPL sample is dominated by the production of one manufacturer, H. Tinsley & Co. If all but ten recent Tinsley SPRTs are removed from the sample, still leaving a group of 60 SPRTs, then the mean (scale-intrinsic) SRI rises from − 0.12 mK to + 0.12 mK (see the final row in Table 1), more in line with other studies. Thus, there is some evidence of production dependence in the sample. Note also that seven of the SPRTs in the sample of Zhiru Kang et al. [6] were from Tinsley, without which the mean value rises from − 0.22 mK to − 0.03 mK.

In other respects, the studies are quite consistent: the low mean values suggest that the ITS-90 W_r values at the fixed points involved are reasonably self-consistent, and the dispersions of the SRI, as characterized by their standard deviations, are in the range 0.29 mK to 0.48 mK.

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