Pramāṇa - J. Phys., Vol. 30, No. 3, March 1988, pp. 245–249. © Printed in India.

Optimization of deconvolution in Compton profile measurements

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MS received 5 August 1987; revised 4 January 1988

Abstract. The method of generalized least squares has been used to deconvolute the Compton profile measurements in nickel. The method depends on two arbitrary parameters namely the cut-off parameter K and the damping factor λ. This has been discussed and a method suggested to optimize the damping parameter.

Keywords. Deconvolution; Compton profile.

PACS Nos 35·80; 34·90; 34·50

1. Introduction

Deconvolution in Compton profile measurements has been the subject of discussion in the past by many investigators. Among the many convolution schemes available in literature, the well-known ones are the Fourier analysis based on Stokes method (Cheng *et al* 1971) and the successive approximation using different kinds of smoothing functions (Reed and Eisenberger 1972) and the method of generalized least squares (Paatero *et al* 1974a). The generalized least squares is the most commonly used method and depends on variable parameters namely those which control the frequency and hardness of cut-off. The cut-off characteristics were discussed in detail by Cheng *et al* (1971). The parameter which controls the frequency is known as damping factor and is taken arbitrarily by different authors. The purpose of this paper is to reinvestigate this damping factor.

2. Experimental set-up and data

In order to calculate the Compton profile we have used the method of generalized least squares, the details of which were given by Paatero *et al* (1974a, b). The K value is usually taken to be 0 or 2 (Towmey 1963) but is taken as 2 in the present analysis. A program for deconvolution based on the above method has been developed on the DEC 2050 computer. The apparatus used for the experimental study of Compton profile consists of various components (see figure 1). The Compton profile of Ni metal is measured using 59·54 keV γ-rays from a 1000 mCi annular source ^{241}Am obtained from the Radio Chemical Centre, Amersham, UK. The experimental set-up consists of a scattering chamber, an intrinsic germanium detector (Canberra model

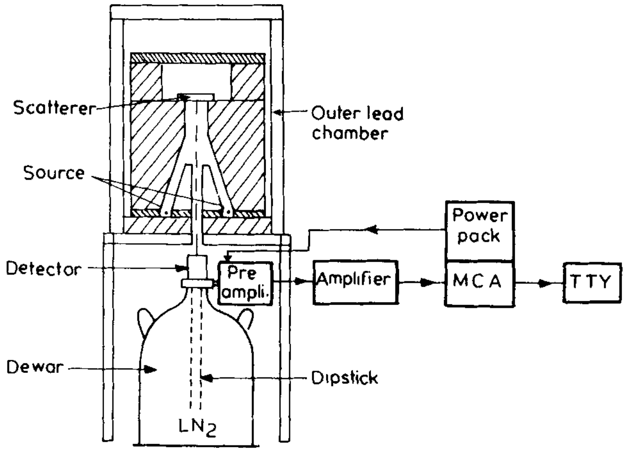

Figure 1. Block diagram of Compton profile experimental set-up.

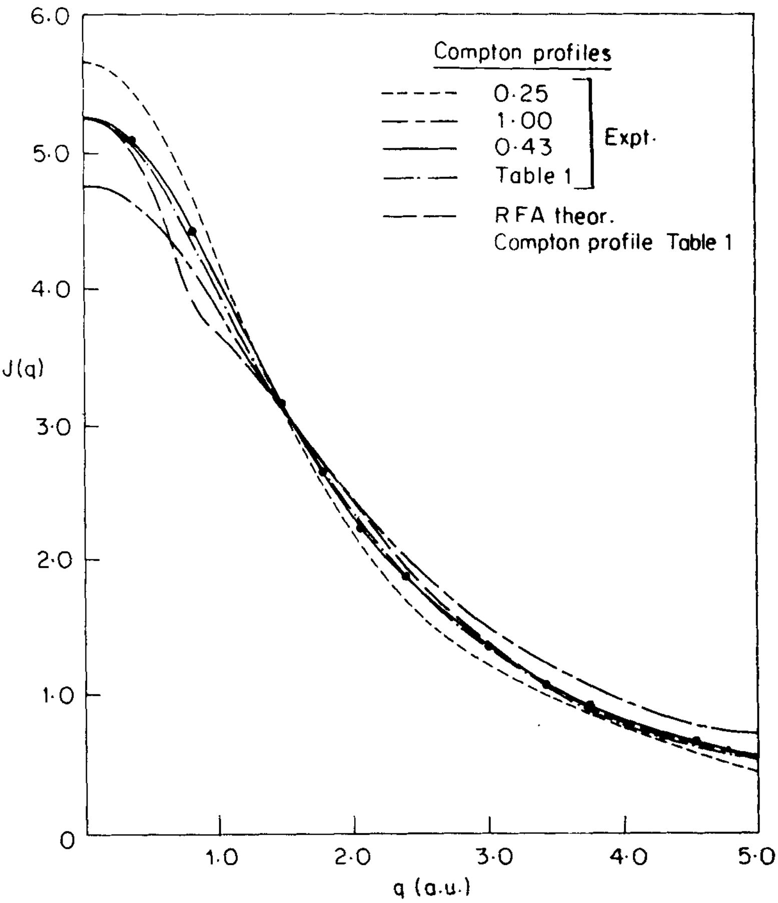

Figure 2. A comparison of present experimental Compton profiles for different damping parameters λ with earlier experimental (Eisenberger and Reed 1974) and theoretical (Berggren *et al* 1977) results.

711005, resolution 200 eV at 5·9 keV), a pre-amplifier, an amplifier and a multi-channel analyser (model series 30 Canberra Inst., USA). The scattering angle is fixed at (165° ± 2·5°) by a lead collimator. The energy scale of multichannel analyser is calibrated using ^{133}Ba source. The background radiations reaching the detector are observed for setting the detector without scatterer. The background thus obtained is properly accounted for in the Compton profile.

The spectrum, as a function of energy, is obtained in the Compton region of interest after substracting the background (channel-wise). Double scattering correction is applied. The peak point of the spectrum is determined and the scattering angle obtained. Using the expression (dq/dE) at each point, the energy spectrum is converted into momentum spectrum to find the Compton profile $J(q)$ as a function of q and this is normalized. Various values of damping parameter λ in the range of 0·25 to 1·0 are taken and the Compton profiles for various damping parameter λ are shown in figure 2.

3. Optimization of damping parameter

The order of the value of λ as given by Paatero *et al* (1974a) is 100–200 or 500. But in the present investigations the values of 0·1, 0·2 etc, which are of the same order, are chosen since the Compton profile is normalized in the present study.

The Compton profile calculated on the basis of the renormalized free atom model (Berggren *et al* (1977), is also plotted in figure 2, as given in table 1, along with the deconvoluted Compton profile $j(q)$ for various values of λ and the experimental results as reported (Berggren *et al* 1977).

In order to understand the optimum value of λ, the difference in $J(q)$(exp) with $J(q)$ (RFA) (for various values of q) is plotted against λ (figure 3). This figure shows that except in the region of q, where free electron description has the usual shape of

Table 1. Compton profile of Ni metal.

q (a.u.)	RFA model calculation (Berggren *et al* 1977)	Experimental results	
		Eisenberger and Reed (1974)	Present
0·0	5·259	5·261	5·250 ± 0·052
0·2	5·170	5·206	5·205
0·4	4·919	5·003	5·049
0·6	4·487	4·687	4·790
0·8	3·897	4·316	4·474
1·0	3·684	3·936	4·102 ± 0·050
1·2	3·471	3·537	3·707
1·4	3·226	3·248	3·316
1·6	2·962	2·934	2·942
1·8	2·693	2·626	2·612
2·0	2·430	2·340	2·315 ± 0·048
3·0	1·402	1·347	1·339 ± 0·045
4·0	0·812	0·772	0·830 ± 0·04
5·0	0·547	0·519	0·551 ± 0·03

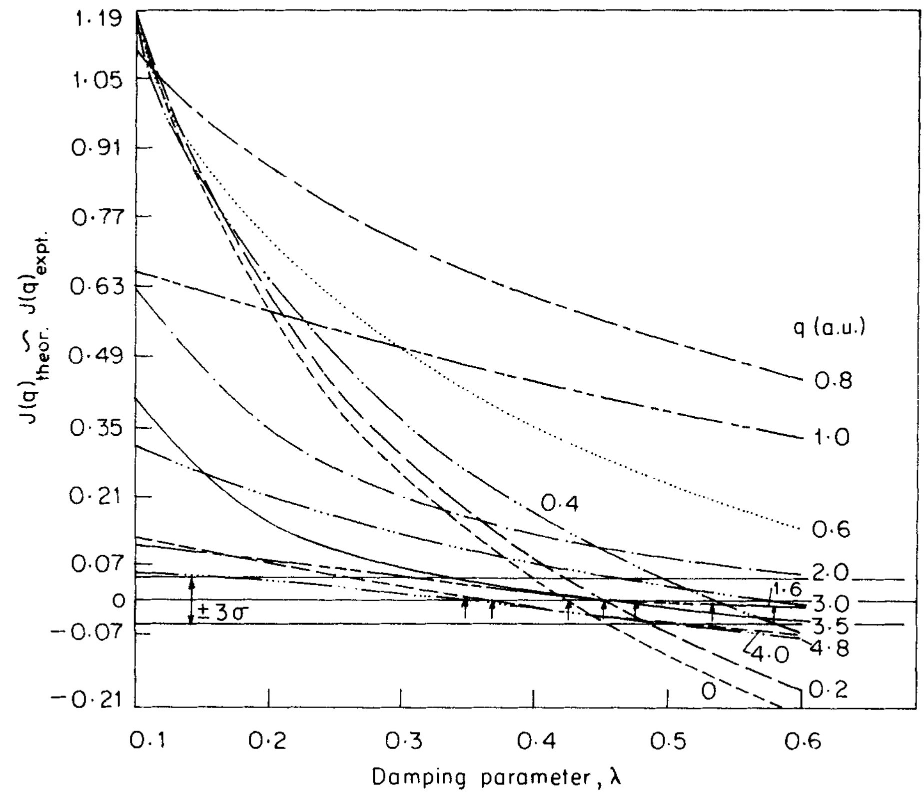

Figure 3. Difference of theoretical (RFA model calculation) and present experimental Compton profiles versus damping parameter λ at different momentum (q) values. The error of $\pm 3\sigma$ in $J(q)_{\text{theor.}} - J(q)_{\text{expt.}}$ is also shown in the graph.

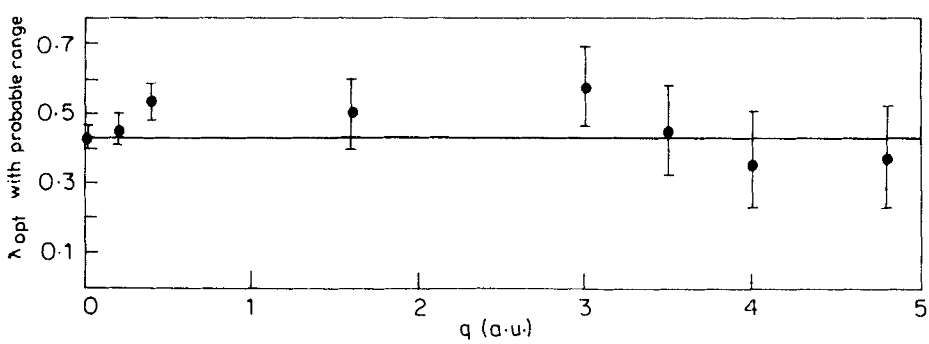

Figure 4. The optimum value of damping parameter λ versus momentum q is plotted and the errors shown are with the range $\pm 3\sigma$.

an inverted parabola with their number determining the Fermi momentum, the difference between theory and experiment is zero for certain λ_{opt} values. Considering the error of $\pm 3\sigma$ in $J(q)$, the range of λ_{opt} values can also be determined. The plot of λ_{opt} (with error) versus q is shown in figure 4 and it is seen that one can assign the mean value of λ_{opt}.

In the theoretical calculation of the Compton profile, the tightly bound core is not affected and generally taken as that given by Biggs *et al* (1975) and therefore λ may be taken by comparing the theoretical Compton profile with the experimental values for core electrons as outlined above.

In the present investigation it is found that from theoretical consideration the optimum value of λ can be taken to be 0·43 for the best fit.

Acknowledgement

One of the authors (VKA) is thankful to the University Grants Commission for financial help.

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