GAMMA- AND X-RAY SPECTROMETRY WITH SEMICONDUCTOR DETECTORS

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Experimental setup

The basic parts of the experimental setup in γ- or X-ray spectrometry are the detector, the electronics and the source of photons. We have devoted sections of this chapter to each of these three components and, in addition, two sections to the source–detector arrangement and recommended test measurements.

2.1 Detectors

2.1.1 General characteristics of photon detectors

Most modern photon detectors rely on a common series of steps in the detection and measurement process. We will describe the general features of these steps only in sufficient detail to understand why different types of detectors have different operating characteristics. The detectors discussed here are the gas detectors, the NaI(Tl) scintillators, and the Ge(Li), high-purity Ge, and Si(Li) semiconductor detectors. Many of these detectors are also used to count electrons and heavy charged particles, but this discussion will be limited to their use as photon detectors. For more extensive discussions of detector characteristics we would recommend the book of Knoll (1979) and the monograph from the National Committee on Radiation Protection, NCRP (1985).

The operation of these detectors involves:
- first, the conversion of the photon energy to kinetic energy of electrons (and positrons) by photoelectric absorption, Compton scattering or pair production;
- second, the production of electron–ion pairs, electron–hole pairs or excited molecular states by these electrons; and
- third, the collection and measurement of the charge carriers or the light emitted in the deexcitation of the molecular states.

Before considering the various detectors, we need to note the characteristics that we wish to compare. As discussed in section 1.1, a photon
Experimental setup

A detector will convert such a line spectrum into a combination of lines and continuous components. As long as the lines are observable they can be used to determine the energies and intensities of the original photons, but if the lines are lost in the associated continua it is usually not possible to determine these quantities. The ability of the detector to produce lines or peaks for monoenergetic photons is characterized by the peak width and the peak efficiency. The width is commonly specified as the FWHM in keV, also called resolution. (The authors acknowledge that the term "resolution" might more properly be directly related to the resolving power or the reciprocal of the peak width. However, the modern practice in this field is not to differentiate between resolution and peak width.) The peak efficiency of the detector is the ratio of the number of counts in the peak corresponding to the absorption of all the photon energy (i.e., in the full-energy peak) to the number of photons of that energy emitted by the source. Both the peak width and the peak efficiency are functions of the photon energy.

In the first of the three processes in the list above, the density of the detector material, its atomic number and its volume will be important. If the material is of low density, low Z and small volume, the probability that a photon will interact will be low, and if an interaction does take place the probability of retaining all the photon energy in the detector will be low. Therefore, the use of such a detector to measure a line spectrum may be limited to low-energy photons. For higher energy photons, the monoenergetic lines may be lost and only a continuum observed. So, such a detector may be useful for counting the number of photons present, but it will be of limited value in measuring an energy spectrum.

A gas counter, typified by an ionization chamber, consists of a volume of gas with an electric field applied across it. Often the gas volume is cylindrical with one electrode being the outside surface and the other a wire along the axis of the cylinder. A typical detector diameter would be 2 or 3 cm, and the gas might be methane or an argon–methane mixture. Thus, these detectors consist of a low-density material and have a moderately small thickness. This means that they have a low efficiency for counting photons and at moderate photon energies (e.g., 200 keV) have a very small probability of absorbing all of the photon energy and producing the line components in the spectrum. However, there are specialized, quantitative uses for these systems. If one wishes to compare the activity of two sources of the same nuclide, this can be done accurately with some forms of these detectors.

In comparison to the gas detectors, the NaI(Tl) scintillation detectors consist of a higher Z material at a higher density and often have a large thickness (typically 8 cm). This means that they have a higher probability of detecting photons and a much higher probability of absorbing all of the photon energy. The detectors are, in fact, quite useful to energies of several MeV.

The Si and Ge semiconductor detectors have the same advantages over the gas detectors as the NaI(Tl) detectors, but they do have a lower Z than the iodine of the NaI(Tl) detectors and are smaller in size. Therefore, as far as the processes in the first step are concerned, they are at somewhat of a disadvantage compared to the NaI(Tl) detectors. Between the Si and Ge detectors themselves, Ge has both a higher Z and a higher density by a factor of over 2 and, therefore, is better for higher energy photons.

For those detectors in which charge, rather than light, is collected, in the second process in the list above, the important quantity will be how many electron–hole pairs or charge carriers are formed. There will be statistical variations in this process, so one expects that, other things being equal, the larger the number of pairs formed the more constant this quantity will be. That is, in the terminology of section 1.1, the width of the lines from monoenergetic radiation will be narrower.

The gas counters and the semiconductor detectors can be compared directly since the semiconductor detectors are essentially solid-state ionization chambers. A major difference between the gas counters and the semiconductor detectors is in the average energy required to produce a charge-carrier pair; for gas detectors this is about 30 eV, and for the semiconductor detectors about 3 eV. From these values one may expect that the spectra from semiconductor detectors will have peaks with a much less statistical broadening. On the other hand, the NaI(Tl) detectors can not be compared directly since their operation depends on the collection of light rather than of charge, but the average energy needed to produce a light photon is about 100 eV.

For the third step in the list above, the collection and measurement of the charge carriers or light, the important properties will depend on the particular type of detector and cannot be generalized except to say that the quality of the detector materials will be important. In fact, the development of each type of detector required the development of methods to fabricate high-quality detector material.

There are other properties that might be compared between detector types, but they are less quantitative. One such property would be the count rate from the background radiation, either the gross rate or the rate in a particular energy region of a spectrum. Also, one might compare the cost of a detector system and the ease of its operation. Although these properties may be important, they will not be addressed here.
2.1.2 Physical processes in semiconductor detectors

Within the scope of this monograph, we can not discuss in depth the fundamental solid-state physics needed to understand in detail the physical processes in a semiconductor detector. Interested readers may consult books on detectors, such as those of Knoll (1979) or Price (1964), or review articles like those of Pehl (1977), Ewan (1979) or Haller et al. (1981). In the following we will only present basic information related to the operational characteristics of the detectors. This includes table 2.1 where the more important properties of single crystals of silicon and germanium are summarized.

In a single crystal of semiconducting material such as silicon or germanium, the sharply defined atomic electron states are broadened into bands of energy states that are characteristic of the crystal as a whole. In the absence of excitation, the outer electrons are bound in an energy band called the valence band. The next highest states lie in the conduction band which is separated from the valence band by an energy known as the band gap. As shown in table 2.1, the band gaps in these crystals are of the order of 1 eV. If no impurities are present, the gap contains no allowed energy

<table>
<thead>
<tr>
<th></th>
<th>Si</th>
<th>Ge</th>
</tr>
</thead>
<tbody>
<tr>
<td>Atomic number</td>
<td>14</td>
<td>32</td>
</tr>
<tr>
<td>Atomic weight</td>
<td>28.09</td>
<td>72.60</td>
</tr>
<tr>
<td>Density (300 K) in g·cm⁻³</td>
<td>2.33</td>
<td>5.33</td>
</tr>
<tr>
<td>Dielectric constant</td>
<td>12</td>
<td>16</td>
</tr>
<tr>
<td>Forbidden energy gap (300 K) in eV</td>
<td>1.115</td>
<td>0.665</td>
</tr>
<tr>
<td>Forbidden energy gap (0 K) in eV</td>
<td>1.165</td>
<td>0.746</td>
</tr>
<tr>
<td>Intrinsinc carrier density (300 K) in cm⁻³</td>
<td>1.5·10¹⁰</td>
<td>2.4·10¹³</td>
</tr>
<tr>
<td>Intrinsinc resistivity (300 K) in ohm·cm</td>
<td>2.3·10⁻²</td>
<td>47</td>
</tr>
<tr>
<td>Electron mobility (300 K) in cm²/V·s</td>
<td>1350</td>
<td>3900</td>
</tr>
<tr>
<td>Electron mobility (77 K) in cm²/V·s</td>
<td>2.1·10⁴</td>
<td>3.6·10⁴</td>
</tr>
<tr>
<td>Hole mobility (300 K) in cm²/V·s</td>
<td>480</td>
<td>1900</td>
</tr>
<tr>
<td>Hole mobility (77 K) in cm²/V·s</td>
<td>1.1·10⁴</td>
<td>4.2·10⁴</td>
</tr>
<tr>
<td>Energy per electron–hole pair (300 K) in eV</td>
<td>3.62</td>
<td></td>
</tr>
<tr>
<td>Energy per electron–hole pair (77 K) in eV</td>
<td>3.76</td>
<td>2.96</td>
</tr>
<tr>
<td>Fano factor (77 K)</td>
<td>0.084</td>
<td>0.08</td>
</tr>
<tr>
<td></td>
<td>0.085 – 0.137</td>
<td>0.058</td>
</tr>
<tr>
<td></td>
<td>0.057, 0.064</td>
<td></td>
</tr>
</tbody>
</table>

* Data are from Knoll (1979).
* Stroken et al. (1971).

states. An electron can be promoted from the valence band to the conduction band by imparting to it an energy at least equal to that of the band gap. While in the conduction band, the electron is free to move under the influence of an externally applied electric field and can be collected at an electrode. The vacancy or hole in the valence band resulting from the electron excitation can also move by the mechanism of electron transfer in a direction opposite to that of the electron. Because the mechanisms for movement of the holes and electrons are different, the speed with which the two charges move through a crystal (i.e., their mobilities) will differ. As shown in the table, at 77 K, the temperature at which these detectors are commonly operated, this difference is a factor of about 2 for Si, but only 15% for Ge. Both electron and hole charges are collected to form the pulse, so the pulse shape (voltage as a function of time) will reflect the differing mobilities.

When a photon interacts in the crystal, bound electrons are excited to the conduction band by the primary electron from the interaction. These secondary electrons, if sufficiently energetic, can create additional secondary electrons. Through this cascading process, the energy of the primary electron is expended in the production of many electron–hole pairs that are then free to be collected at the electrodes of the device. To collect this charge, an electric field of about 1000 V/cm is needed. The manufacturer will generally recommend a bias voltage for each detector. This voltage is chosen low enough to minimize the probability for a voltage breakdown, but high enough to provide good charge collection and thereby good peak shapes.

Since in practice the semiconductor material is not free of impurities or crystal defects, its operation as a photon detector is more complex. One effect of impurities with three valence electrons, such as boron, aluminum, gallium or indium, is the introduction of free holes within the crystalline structure. These are called acceptor impurities since the holes can accept electrons. Similarly, impurities with five valence electrons, such as phosphorus, arsenic and antimony, introduce free electrons. These are called donor impurities, since they donate electrons. Materials in which the acceptor impurities predominate are referred to as p-type materials, those with primarily donor impurities as n-type materials.

An electric field applied across such a crystal results in an electric current based on the presence of these holes or electrons, and the statistical variations in this current represent a noise level above which the pulses for photon interactions must be detected. For the material available in the early days of semiconductor detectors, the noise level from the presence of acceptor impurities would totally mask the pulses from any photon. To reduce this steady-state current to an acceptable level, it was necessary to
create an intrinsic region within the crystal, devoid of free charge carriers. This was done by drifting lithium ions into the germanium material. The lithium was deposited on the upper surface of the p-type crystal and drifted through the larger part of its volume. Lithium, an interstitial donor impurity, will, on a one-to-one basis, compensate the acceptor impurities, creating the intrinsic region. This is what is called a lithium-drifted germanium, or Ge(Li), detector. The structure of a planar detector of this type is illustrated in fig. 2.1a. The excess lithium on the upper surface resulted in a highly doped n⁺ layer which served as an electrical contact, and a thin uncompensated layer remained on the opposite side. In such a detector, the lithium will continue to drift significantly at room temperature; therefore, the detector must be kept cold (usually at liquid nitrogen temperature) at all times, even during shipping.

For sufficiently pure germanium material, the desired intrinsic region can also be achieved directly without compensation by the creation of a diode structure. This structure may be obtained by evaporating lithium on one surface of the p-type germanium and allowing it to diffuse into the germanium for a short time period, and a short distance. A reverse bias applied to this n⁻-p junction pushes the majority carriers from the junction on both sides, creating the intrinsic region. The process of recession of the free charges proceeds on both sides of the junction until the electrostatic field induced by charged atoms balances the field from the externally applied electric potential. The thickness of the depletion layer is related to the applied voltage and the impurity concentration in the material. A detector made in this way is called an intrinsic or high-purity Ge detector and is illustrated in fig. 2.1b. In contrast to the Ge(Li) detectors, the high-purity Ge detectors can be stored and transported at room temperature.

The lithium-drifted Ge detectors were made from material with of the order of 10¹² impurity atoms per cm³, but this material was not pure enough to make the high-purity type detectors. The latter detectors need material in which the number of acceptor sites minus the number of donor sites is of the order of 10⁹ cm⁻³, and improvements in the production of germanium crystals have made this possible. For a discussion of the impurities in Ge and Si material, especially for high-purity detectors, see Hall and Soltes (1971), Hansen (1971) and several articles in the symposium proceedings edited by Haller et al. (1983).

In addition to the electrons that are excited to the conduction band by photon interactions, electrons are excited there thermally, and this mode of excitation produces a statistical noise background. To minimize this noise, semiconductor photon detectors must be operated at reduced temperatures. The highest temperature at which acceptable operation is possible is dependent upon the type and abundance of crystal impurities and defects. Although acceptable operation has been achieved over a sizable temperature range, a practical operating temperature is 77 K, the temperature of boiling nitrogen, since this temperature can be achieved readily by use of liquid nitrogen as the refrigerant.

2.1.3 Resolution

As noted above, the two main quantities of interest for a detector are its efficiency and its resolution. The former depends primarily on the size and shape of the detector; these parameters will be discussed in section 2.1.4. The factors that influence the width of the peaks (FWHM) or the resolving power of the detector are:

- the statistics of the charge-creation process,
- the properties particular to the individual detector, primarily the completeness of the charge collection process, and
- the electronic noise.

The first of these contributions to the peak width is inherent to each detector material. The band gap in single-crystal germanium is 0.67 eV at 77 K, but an average energy $e = 2.96$ eV (Pehl et al. 1969 and table 2.1) is required to create a free electron–hole pair in Ge, and $e = 3.76$ eV is needed in Si. The extra energy is dissipated in the creation of lattice phonons. Although the average number of pairs is $N = E/e$, the division of the photon energy between the different excitation modes causes a
statistical distribution in the number of pairs, and thus a statistical spread of the amplitudes of the pulses produced by a monoenergetic group of photons that are completely absorbed in the detector volume. If the individual pairs were independently created, Poisson statistics would apply and the standard deviation of the distribution of \( N \) would be \( \sqrt{N} \) (as discussed in section 1.5.1). However, the statistics of the creation of the electron–hole pairs is not Poisson, but rather is described according to a theory proposed by Fano (1946). In this description, the observed root-mean-square deviation in the number of pairs is expressed as \( (F \cdot N)^{1/2} \) where \( F \) is the Fano factor. From this expression it follows that this contribution to the observed peak width is

\[
w_i = 2.355 (F \cdot E_i \cdot e)^{1/2}.
\]

(2.1)

Since there is no satisfactory theory for the calculation of the Fano factor, it must be measured for each detector material. This factor is an inherent property of the material, so there is only one value for Ge and one for Si. The major experimental difficulty in its determination is that all other factors that increase the resolution, such as electron and hole trapping and electronic noise, must be eliminated or measured and subtracted. As indicated in table 2.1, the Fano factors for germanium and silicon are about 0.06 and 0.08, respectively. The good resolution of semiconductor detectors depends directly on the fact that these values of \( F \) are much smaller than 1.0. Note that this contribution to the peak width increases as \( E_i^{1/2} \).

The next contribution to the photon peak width is a characteristic of each detector and depends primarily on the loss of charge carriers. The most important processes responsible for incomplete collection of the free electrons and holes is charge trapping (Armantrout and Thompson 1970). Trapping occurs when a charge is trapped in one of the states introduced into the energy gap by impurities or crystal imperfections. Further excitation is required to release the trapped charge and allow it to be collected. The mean time a charge carrier remains in the trap is a function of the energy of the trapping state, the temperature and the electric field. The first two parameters are fixed by the characteristics of the particular crystal and the standard cooling method, but the bias voltage is an adjustable variable. Because increasing the voltage improves the charge collection, it is normally set near the maximum voltage the detector will take without risk of a voltage breakdown. Both acceptor and donor traps exist within crystals so that each type of charge carrier may be trapped.

Trapping can cause either a complete loss of this charge or just a slowing of the rate of charge collection. The loss of the charge creates a low-energy asymmetry or tailing on the peaks in the photon spectrum. Trapping characteristics may vary with position in the detector due, in part, to the nonuniformity of the electric field, especially in a closed-end coaxial geometry (discussed below). This means that a large fraction of the pulses in the low-energy tail of a full-energy peak may come from a particular region of a detector; for example, the front corners of a closed-end coaxial detector where the electric field is low. This suggests that one can improve the peak shape, and possibly the resolution, by the rejection of slow rise-time pulses. This low-energy tailing may increase the FWHM of the peaks, or it may only influence the peak shape below the half-maximum height. As discussed in section 3.3.3, the tailing may have a significant influence on the data analysis methods even if it does not influence the FWHM value.

From their experience, the commercial detector manufacturers have developed practical methods to minimize the influence of trapping and

![Table 2.2](image)

Typical detector sizes and resolutions from manufacturers' literature.

<table>
<thead>
<tr>
<th>Type</th>
<th>Size</th>
<th>Resolution (keV)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Si(Li)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Area (cm²)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.12</td>
<td>5.9</td>
<td>122</td>
</tr>
<tr>
<td>0.28</td>
<td>0.16-0.17</td>
<td></td>
</tr>
<tr>
<td>0.80</td>
<td>0.17-0.18</td>
<td></td>
</tr>
<tr>
<td>2.0</td>
<td>0.18-0.19</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.22-0.25</td>
<td></td>
</tr>
<tr>
<td>Ge planar</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Depth (cm)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Diameter (cm)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.5</td>
<td>0.6</td>
<td>0.145</td>
</tr>
<tr>
<td>0.5-1.0</td>
<td>1.0</td>
<td>0.24-0.18</td>
</tr>
<tr>
<td>0.5-1.6</td>
<td>1.6</td>
<td>0.29-0.20</td>
</tr>
<tr>
<td>0.5-1.3</td>
<td>2.5</td>
<td>0.46-0.30</td>
</tr>
<tr>
<td>1.0-1.5</td>
<td>5.1</td>
<td>0.62-0.54</td>
</tr>
<tr>
<td>Ge coaxial</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Efficiency (%)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>n-type</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td></td>
<td>0.66-0.74</td>
</tr>
<tr>
<td>20</td>
<td></td>
<td>0.69-0.79</td>
</tr>
<tr>
<td>30</td>
<td></td>
<td>0.72-0.84</td>
</tr>
<tr>
<td>p-type</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td></td>
<td>0.82-1.0</td>
</tr>
<tr>
<td>20</td>
<td></td>
<td>0.85-1.1</td>
</tr>
<tr>
<td>40</td>
<td></td>
<td>0.88-1.2</td>
</tr>
<tr>
<td>50</td>
<td></td>
<td>0.90-1.2</td>
</tr>
</tbody>
</table>

\(^{a}\) The resolution ranges are given for the ranges in the depth and in the same order; that is, the resolution improves as the depth increases.

\(^{b}\) Efficiency at 25 cm relative to that of a 7.6-cm × 7.6-cm NaI(Tl) detector at the same distance.
thereby to produce quite reasonable peak shapes. In spite of this, there is still interest in these effects at the research level as illustrated by recent articles on the effect of trapping on the resolution, the peak shape and timing by Katkov and Krupman (1983), Simoen et al. (1986) and Morozov et al. (1986). These authors also discuss the differences in the effects of hole and electron traps and of traps of different depths.

Although the electronics used with these detectors will be discussed in section 2.2, to complete the list of contributions to the peak width, we note that the electronic system also introduces a noise level. This contribution depends primarily on the leakage current of the detector and its capacitance; it is independent of the photon energy and uncorrelated with the two terms from the detector noise. Each of these three terms has a Gaussian distribution, so their widths add in quadrature. The square of the total peak width is then

\[ w^2 = w_i^2 + w_x^2 + w_e^2 \]  

(2.2)

where \( w_x \) is the contribution from the detector influences such as trapping and \( w_e \) that from the electronics. Some typical values of observed peak widths are given in table 2.2. They vary from 0.16 to 2.5 keV for various detector configurations and photon energies. Since the values in the table are from commercial literature they tend to be values that are guaranteed, and the measured values will be somewhat smaller. In the table it is noted that for planar detectors the resolution improves as the depth increases; this is a result of the decrease in detector capacitance with a decrease in the diameter/depth ratio.

2.1.4. Detector configurations

Germanium and silicon semiconductor detectors have been produced successfully in several shapes and in a range of sizes. Detector sizes, and indirectly their shapes, have been determined, first by the maximum size of the available blocks or ingots of pure germanium or silicon material, and second by the depth to which an intrinsic region can be formed in the manufacturing process. Therefore, different detector shapes became available as different semiconductor material and manufacturing techniques were developed.

Si(Li), Ge(Li) and high-purity Ge detectors have been made in the planar geometry shown in fig. 2.1. Ge(Li) detectors were also made in the first two geometries illustrated in fig. 2.2 and high-purity Ge detectors are available in the last three of these configurations. The first detectors were of the planar type because this was the simplest to make. The diameter of these detectors was limited by the ingot size and the thickness by the inability to make a Li-drifted detector thicker than 7 to 10 mm. Next, the true-coaxial geometry was developed in order to increase the detector volume within this limit on the Li-drift depth. Lastly, the closed-end geometry provides for a larger sensitive volume for a given volume of material, and at the same time for an increase of the detector efficiency by increasing the sensitive volume near the source. With the availability of high-purity p-type germanium the drifted detectors were gradually replaced by the high-purity germanium detectors. A few years ago high-purity, n-type detector material became available and is used to make closed-end coaxial detectors with thin entrance windows (Raudorf et al. 1979). The well detectors were developed in order to obtain a very high efficiency for sources that are small enough to be placed inside the well. All of these detector geometries are still in use since each has advantages for particular types of measurements. Table 2.2 gives the range of sizes that are routinely available commercially for semiconductor detectors in the various geometries.

The electric field in the detector is produced by placing an external voltage between two electrically conducting detector surfaces that are separated by a passive or nonconducting detector surface area. For a
discussion of the theory of such contacts, see Goulding (1966) and Pehl (1977). Several types of electrical contacts have been used, such as a P- or Li-diffused layer for one contact and an evaporated or ion-implanted metal film for the other. The diffused contact is an n⁺ layer and is the positive electrode, and the metal contact is a p⁺ layer and is the negative electrode. Inherently the diffused contact will be thick, and the metal contact will be quite thin; for example, on some modern detectors a Li-diffused contact of 600 μm is used along with a boron ion-implanted contact of 0.3 μm. These contacts are indicated in figs. 2.1 and 2.2. They produce a layer of attenuating material, from which the charge carriers are not collected, and are therefore called dead layers. For planar high-purity Ge detectors, the thin contact is at the front surface so that low-energy photons can reach the sensitive volume. For p-type coaxial Ge detectors, the diffused contact is on the outside surfaces, and this limits their useful energy range to above about 40 keV. In contrast, an n-type coaxial detector has a very thin front contact and is usable down to 5 keV (Raudorf et al. 1979). When low-Z materials like lithium and boron are used for these contacts, the high-energy fluorescence X rays, which are present when a metal such as gold is used, are eliminated.

In the planar configuration the electric field is nearly uniform throughout the depletion region and, in principle, this has the advantage of producing uniform and good charge collection. However, there may be changes with time in the charge collection properties at these edges. Planar detectors can be made in a variety of thicknesses and this allows an optimization for the planned measurements. If we are interested in counting only low-energy photons, say below 80 keV, we can use a thin detector and thereby reduce the spectral background from high-energy photons.

Among the larger detectors, the open-end coaxial units have electric fields that are uniform in the axial direction. This uniformity allows better timing characteristics for coincidence measurements. The detector surfaces that are not electrodes must be carefully prepared. There can be a leakage current along the surface that will influence the performance of the detector, and the magnitude of this current will depend on the proper surface treatment. One advantage of the closed-end coaxial geometry is that it minimizes this surface area.

In summary we show in fig. 2.3 typical full-energy-peak efficiency curves for detectors of different types. These curves show the differences due to the size for coaxial detectors and the low-energy difference between the p-type and n-type configurations. There is no inherent difference between the efficiency of coaxial Ge(Li) and p-type Ge detectors, as long as they are of the same size.

2.1.5. Detector mounting

Since essentially all modern detectors come from commercial manufacturers, we normally do not have to be concerned about the methods used to mount them. However, some basic ideas may be worth mentioning. A typical detector assembly is shown schematically in fig. 2.4 and photographically in fig. 2.5. The detector assembly must provide:
- cooling of the detector,
- a high-quality vacuum,
- suppression of heat transfer,
- mounting for the electrical contacts,
- isolation from external vibration, and
- an entrance window for photons.

Detector cooling has normally been achieved with the detector mounted on one end of a metal rod, while the other end protrudes into the tank of liquid nitrogen. Although one usually uses a large liquid-nitrogen dewar system with a capacity of up to 30 l, there are now detectors with small dewars that hold only a few liters of liquid nitrogen and are intended to stay cold for a few hours or a day. The latter detector systems are small enough to be portable, so field measurements can be made easily. If warming-up of the detector is planned or can not be avoided, the detector bias must be taken off before the detector temperature rises significantly. Recently electrically powered cryogenic refrigerators have been developed that can cool a Ge detector (Kromer et al. 1985).
The high-quality vacuum is necessary to minimize the collection of contaminants on the detector surfaces which cause degradation of the performance. Contamination of the insulating surfaces of the detector can result in a voltage breakdown. This vacuum is provided at the factory by pumping the mount and placing some absorbant material (like a molecular sieve) in the system to trap gases that accumulate in the mount at later time. In most cases the first stage or stages of the preamplifier are also mounted in the vacuum.

Since the outside of the detector assembly is at room temperature and the detector is at or near 77 K, a thermal shield is needed to prevent the transfer of heat from the outer surfaces to the detector. The vacuum acts as a shield against conductive and convective heat transfer, and reflective materials are used as shields against radiative transfer.

The mount must provide the necessary electrical contacts and insulation. All detectors have a bias across them, and in some cases this may exceed 4000 V. With such a large voltage it is necessary that the system be carefully designed to prevent a voltage breakdown anywhere in the system. Such a discharge can easily damage the transistors in the front end of the preamplifier and thereby require that the vacuum system be opened to make repairs and to recondition the detector surfaces. Such reconditioning will usually change the characteristics of the detector to the extent that it must be recalibrated.

The mounting system should also provide an environment which isolates the detector and its electronics from external vibrations (i.e., the system should not be microphonic). If this is not the case, such vibrations can
cause large spikes of noise that prevent the observation of the photon induced pulses and which will produce extraneous counts in the spectrum.

There is one feature of the mounting system that directly influences the efficiency of the detector. This is the photon attenuation in the front window of the mount. This window is usually constructed of aluminum or beryllium, but in special cases may be made of copper or other material. Beryllium is used in order to minimize the photon attenuation at low energies, especially on Si(Li), planar Ge and n-type coaxial Ge detectors. Copper and magnesium have been used recently for systems in which it is desired to minimize the background radiation from the detector materials (see section 5.3.1). In table 2.3 the typical thicknesses of beryllium and aluminum used for commercial systems are given along with the photon attenuation. In the future other materials may be used in special cases as evidenced by the recent suggestion of Rimbert and Testard (1986) to use a multilayer composite of high-purity aluminum interleaved with polyimide films in place of thin beryllium. They argue that beryllium degrades due to corrosion in the air and that it contains impurities, such as U, that are undesirable in some applications.

<table>
<thead>
<tr>
<th>Material</th>
<th>Thickness (μm)</th>
<th>Transmission factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>Be</td>
<td>7.5</td>
<td>0.0003</td>
</tr>
<tr>
<td></td>
<td>12.5</td>
<td>0.0005</td>
</tr>
<tr>
<td></td>
<td>25</td>
<td>0.001</td>
</tr>
<tr>
<td></td>
<td>50</td>
<td>0.002</td>
</tr>
<tr>
<td></td>
<td>125</td>
<td>0.005</td>
</tr>
<tr>
<td></td>
<td>250</td>
<td>0.010</td>
</tr>
<tr>
<td></td>
<td>500</td>
<td>0.020</td>
</tr>
<tr>
<td>Al</td>
<td>25</td>
<td>0.001</td>
</tr>
<tr>
<td></td>
<td>50</td>
<td>0.002</td>
</tr>
<tr>
<td></td>
<td>125</td>
<td>0.005</td>
</tr>
<tr>
<td></td>
<td>250</td>
<td>0.010</td>
</tr>
<tr>
<td></td>
<td>500</td>
<td>0.020</td>
</tr>
</tbody>
</table>

*a* Special order for Si(Li) with small diameter windows.
*b* Standard for Si(Li) with windows of diameter ≤ 1 cm.
*c* Standard for Si(Li) with windows of diameter ≥ 1 cm.
*d* Standard for planar Ge detectors with windows of diameter ≤ 2 cm.
*e* Standard for planar Ge detectors with windows of diameter of about 3 cm.
*f* Standard on planar Ge detectors with windows of diameter ≥ 4 cm and n-type Ge coaxial detectors.

![Fig. 2.6](image)

The liquid nitrogen dewar and the cryostat are made in many configurations, a few of which are illustrated in fig. 2.6. These configurations have been developed to allow the user to place the detector in the position needed for his experiment. The configurations with long cold fingers allow the detector to be placed in a location, or inside an object, where the liquid-nitrogen dewar would prevent its placement with the more common short-necked versions. With these long-necked detectors, one may need to be especially concerned about the quality of the vacuum due to the large internal volume, and about microphonics due to the greater possibility of vibration with the large arm.

2.1.6. Detector influences on pulse amplitudes

Above we have discussed items that are of interest in all situations. Now we wish to turn to a topic that is important only to those who are interested in making very precise γ-ray energy or energy-difference measurements. It concerns influences that occur in the detector and cause small, less than 0.2 keV, shifts in the peak positions. The amplitude of an amplifier pulse, or the equivalent position of a γ-ray peak, depends primarily on the energy of the γ rays and the gain of the electronic system. But, it also depends to a small extent on the details of the interactions in the crystal. There are two
influences that have been described in the literature. The first is a direct result of the electric field in the detector and, therefore, has been called the field-increment effect (Gunnink et al. 1968 and Heath 1969). The second results from the variation of the charge collection over the detector volume (Sakai 1968).

First, let us consider the field-increment effect for the simple geometry of a planar detector. For a γ ray which interacts with the detector by the photoelectric or Compton process, energetic primary electrons are produced which in turn produce electron-hole pairs that are collected to produce a pulse. Since the energy of the primary electrons will be increased or decreased by the acceleration or deceleration in the electric field of the detector, the pulse amplitude will be altered thereby. The average amount of change in the electron kinetic energy will depend on the average direction of the electron path relative to the direction of the electric field.

Although the angular distribution of the primary electrons will be approximately isotropic for low-energy photons, at a few hundred keV the distributions will be peaked in the direction of the incident γ rays. Therefore, for γ rays of higher energy that enter a planar detector through the negative-voltage contact, on the average the detector bias will increase the energy of the primary electrons. For a primary electron with a range of 1 mm and a field strength of 250 V/mm, the maximum effect would be a shift of +0.25 keV. In the actual case, the primary electrons will have a distribution of directions with respect to the original γ rays, so the average effect will be much smaller than this value. This distribution of the values of the acceleration will result in some broadening of the observed peaks, as well as a shift in the peak position.

For a source placed beside a planar detector, the primary electrons that travel in the forward direction will travel perpendicular to the electric field, and their distribution will be approximately symmetric with respect to that field. Therefore, the field-increment effect should be essentially zero.

The field-increment effect will be quite different for γ rays above 1022 keV that interact by pair production (Gunnink et al. 1968 and Heath 1969). Since the primary electron and positron have similar (although not identical) directions of travel, ranges, angular distributions and energy distributions, the acceleration of the two particles will be almost opposite, so the net effect should be much smaller than that for a photoelectric or Compton interaction. This means that double- and single-escape peaks (which must involve a pair-production interaction) will have a relatively small shift compared to a full-energy peak of the same energy when the γ rays enter the detector parallel to the electric field.

The same effect occurs in the coaxial detectors. For an open-end coaxial detector with the source on axis and at a large distance, the γ rays enter the detector perpendicular to the electric field; therefore, the peak shifts should be small. For a closed-end coaxial detector the situation is more complex. For a source on the axis, the angle between the γ ray and the electric field varies from parallel at the center of the front surface to perpendicular near the back surface. Thus, the average effect may be small or large depending on the spatial distribution of the interactions.

There is also an influence on the apparent peak energy from the spatial variation of the charge collection. Sakai (1968) has investigated this effect in two open-end coaxial detectors by measurements with collimated γ-ray beams. He related the results to the expected variation in electron and hole trapping that results from the $r^{-1}$ variation of the electric field. For closed-end coaxial detectors the situation will be more complex since the variation of the electric-field strength is even larger, especially since the electric fields will be low in the front corners of the detector. For planar detectors the variation in the electric fields will be much less and, therefore, to the extent that this effect is based on a variation of the electric field, it should be quite small. However, if there are charge-collection variations over the detector volume due to other causes, there would be a similar effect.

Since these two effects cause changes in the apparent peak energies as a function of the source position, they are discussed in more detail in section 3.5.2.2.

### 2.1.7 Detector specifications

We wish to collect in this section information about the quantities used in the specifications for semiconductor detectors. Typical values for these quantities, as quoted by the manufacturers, are given in tables 2.2 and 2.4. In section 2.5 we discuss in detail how to check the detector performance against these specifications.

#### Resolution (FWHM)

The resolution, or the full width of the peak at one-half of the maximum height above any underlying continuous spectral background for a particular group of monoenergetic photons, is usually specified at energies that are typical for the useful energy range of the detector. These energies are:

- $5.9 \text{ keV (Mn K X rays from } ^{55}\text{Fe) for Si(Li), planar and n-type Ge detectors;}$
- $122 \text{ keV (γ rays from } ^{55}\text{Co) for planar and n-type Ge detectors; and}$
- $1332 \text{ keV (γ rays from } ^{60}\text{Co) for coaxial Ge and Ge(Li) detectors.}$
Experimental setup

Table 2.4

Peak-to-Compton ratios and peak-shape parameters from commercial literature for coaxial detectors of both p- and n-type germanium. All data are for a 1332-keV peak.

<table>
<thead>
<tr>
<th>Efficiency relative to NaI(Tl) (%)</th>
<th>FWHM (keV)</th>
<th>Peak-to-Compton ratio</th>
<th>FWTM/FWHM</th>
<th>FWFM/FWHM</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>1.75</td>
<td>41:1</td>
<td>1.90</td>
<td>2.65</td>
</tr>
<tr>
<td>20</td>
<td>2.0</td>
<td>34:1</td>
<td>2.00</td>
<td>3.00</td>
</tr>
<tr>
<td>20</td>
<td>1.8</td>
<td>51:1</td>
<td>1.90</td>
<td>2.65</td>
</tr>
<tr>
<td>30</td>
<td>2.0</td>
<td>44:1</td>
<td>2.00</td>
<td>3.00</td>
</tr>
<tr>
<td>20</td>
<td>1.9</td>
<td>56:1</td>
<td>1.95</td>
<td>2.80</td>
</tr>
<tr>
<td>40</td>
<td>2.2</td>
<td>46:1</td>
<td>2.00</td>
<td>3.00</td>
</tr>
<tr>
<td>30</td>
<td>1.95</td>
<td>60:1</td>
<td>1.90</td>
<td>2.65</td>
</tr>
<tr>
<td>50</td>
<td>2.2</td>
<td>54:1</td>
<td>2.00</td>
<td>3.00</td>
</tr>
<tr>
<td>2.1</td>
<td>2.5</td>
<td>58:1</td>
<td>2.00</td>
<td>3.00</td>
</tr>
</tbody>
</table>

**FWTM/FWHM**

The peak shape is often specified in terms of the FWTM/FWHM and FWFM/FWHM ratios where FWTM is the full width of the peak at 1/10th of the maximum height and FWFM is the full width of the peak at 1/50th of the maximum height above any underlying continuum. For a pure Gaussian these ratios are FWTM/FWHM = 1.82 and FWFM/FWHM = 2.38, compared to the best values of 1.90 and 2.65, respectively, in table 2.4.

**Efficiency and size**

The size or volume of a detector is specified in different ways depending on its configuration. For planar detectors one specifies the actual thickness and diameter of the detector, which may differ slightly from the sensitive thickness and diameter. In this case the detector thickness is of prime importance since it directly influences the energy beyond which the efficiency starts to decrease sharply. The diameter affects the resolution and the efficiency (at a given source distance).

For large detectors the volume is commonly quoted in terms of the detector efficiency relative to that of a 7.62-cm by 7.62-cm NaI(Tl) detector. To report the efficiency in terms of a NaI(Tl) detector is not a propitious habit and has to be understood historically. This terminology gives the unjustified impression that the NaI(Tl) detector is some sort of fundamental detector against which others have to be compared. This is, of course, not true, and many users of semiconductor detectors will not have available such a detector for comparison purposes. But, as discussed in section 2.5, a NaI(Tl) detector is not needed for checking the specified efficiency. Although this relative quantity cannot be uniquely related to an actual detector volume, this practice of quoting a relative efficiency has the advantage that it eliminates any question about the relationship of the sensitive volume and the total volume of the detector.

The customer might be better served if manufacturers would quote the whole efficiency curve for some standard measuring geometry. Instead, they have confined themselves to the presentation of the typical shapes of the curve for various detector types. Such curves have been reproduced in fig. 2.3.

**Pea-to-Compton ratio**

The peak-to-Compton ratio is defined as the ratio between the maximum amplitude in a peak at 1332 keV and the mean amplitude of the Compton distribution for a ^60^Co source between 1040 and 1096 keV. This ratio increases as the detector size increases (since more Compton-scattered photons are absorbed and contribute to the full-energy peak) and as the resolution improves (since the peak is narrower and therefore higher).

2.1.8 Detector selection criteria

We will comment briefly on the items that need to be considered in the purchase of a semiconductor detector. These items include:
- detector material – Si(Li), p-type Ge or n-type Ge;
- detector configuration (planar, coaxial or well);
- detector volume or thickness and area;
- cryostat and dewar configuration;
- window material and thickness;
- resolution;
- peak shape in terms of FWTM and FWFM at 1332 keV; and
- peak-to-Compton ratio.

The first choice is the type of detector material. For measurements of photons with energies that are below, say, 100 keV, the choice should be between a Si(Li) or a thin planar Ge detector. Si(Li) is usually the better choice for measurements below 20 keV.

For measurements of higher energy photons, one will presumably choose a coaxial Ge detector, either open- or closed-end. In the past we needed to choose between Ge(Li) and Ge detectors, but Li-drifted detectors are no longer readily available. When considering the choice between a p-type or n-type detector, we should note that, at least at the current time, the n-type detectors are more expensive and will have more coincidence summing with low-energy photons. On the other hand, their thin frontal dead layer allows
one to measure both high- and low-energy spectral regions with the same
detector. The n-type detectors have a distinct advantage in cases where the
detector will be exposed to particle radiation, in particular fast neutrons,
which causes deterioration of the detector. The principal damage is due to
the production of hole traps. The holes are collected at the outer electrode
of an n-type detector, and at the inner one on a p-type detector. Since the
major portion of the germanium volume is nearer to the outer electrode, the
holes are more effectively collected in the n-type detector, and the damage
is less apparent in the detector performance.

Next we need to determine the desired size of the detector. For low-energy
measurements this is done by choosing the thickness to optimize the
efficiency cutoff at the higher energies. The area or diameter can be chosen
to obtain the desired resolution or efficiency at a given source distance. For
high-energy photons one quite often wants the largest detector one can
obtain. But, since an increase in size means an increase in price, this choice
is a matter of individual judgement. We have also to keep in mind that the
background count rate increases with the detector size. This is a fact of
particular importance for low-energy measurements. If the radiation of
interest is absorbed in the first few millimeters of the detector material, the
rest of this material is of no use and only provides background. Table 2.2
indicates the range of sizes that are currently available in commercial
detectors of different types. Occasionally still larger sizes [up to 70%
efficiency relative to NaI(Tl)] are offered.

The next choice is the configuration of the cryostat and dewar. We must
consider any structures that the detector arm must avoid, the shielding
required around the detector or around the whole dewar, the shapes of the
sources to be investigated and how the corresponding efficiencies are to be
generated. Horizontal mounts have the advantage that the source can
usually be placed at distances up to several meters from the detector and
that the detector can be placed next to most experimental facilities.

The selection of the window material and thickness must be made to fit
the planned measurements. Some of the choices that are commercially
available are indicated in table 2.3. For the low-energy detectors, Si(Li),
planar Ge and n-type Ge coaxial detectors, the window will normally be
beryllium. The thickness needs to be chosen so that the lowest energy
photons of interest can reach the detector, and thick enough to operate
without significant risk of damage in the planned environment. For other
Ge detectors the window will generally be aluminum. Any standard thick-
ness should suffice for a p-type detector since its thick dead layer prevents
counting photons with energies much below 40 keV. The purchaser should
be very careful to make sure that the dead layer on the detector and the
window thickness are coordinated.

Next one should specify the desired resolution and provide some limitation
on the tailing. Table 2.2, which shows the resolution values quoted in
some commercial advertising, suggests that most of the available coaxial
detectors have very similar resolutions, with a slight increase in peak width
with increasing detector volume. If a decision has fallen in favor of an
n-type coaxial detector only to be able to record low-energy and high-energy
photons with the same detector, one should realize that the resolution
at 5.9 keV is worse by a factor of 3 to 4 than with a Si(Li) or planar Ge
detector. So, if good resolution is important for both energy regions, two
different detectors should be obtained.

A limitation on the tailing is usually made by specifying an upper limit
on the ratio FWTM/FWHM. In case the quality of the peak shape is very
important, one may also specify the FWHM/FWHM ratio. Values of these
ratios that are quoted in some commercial literature are given in table 2.4.
The data in this table indicate that generally the best FWTM/FWHM ratio
is obtained for detectors with the best FWHM.

One should be aware that commercial specifications commonly give the
resolution for measurements with a long (say, 6 μs) amplifier time constant.
If one needs to make measurements with count rates of over, say, 2000 s⁻¹,
one should consider the use of shorter amplifier time constants (2–4 μs).
This will normally result in wider peaks, and one may wish to have the
detector manufacturer quote the resolution at the amplifier time constant
of interest.

The peak-to-Compton ratio increases, or improves, as the detector size
increases and as the resolution improves. Therefore, once one has specified
the detector size and the resolution, the peak-to-Compton ratio is probably
determined. But, one may still wish to specify a lower limit on this ratio.

2.2 Electronics

The electronics system for a semiconductor-detector spectrometer is
shown schematically in fig. 2.7. The system consists of a detector bias
supply, preamplifier, amplifier, analog-to-digital converter, a data storage
device, a pulse generator if desired and possibly a computer. A survey of
the commercial literature shows that a great variety of electronic modules
are available. This literature should be a sufficient guide in the selection of
components unless the planned measurements have some unusual char-
acteristics, such as very high-count rates or operation in an environment
with a wide temperature range. In addition to the specific references in the
text below, articles on all of the electronic components are given in the
conference proceedings edited by Brown et al. (1969). Readers interested in
the fundamentals of the electronics are referred to textbooks like those of Kowalski (1970), Weinzierl and Drgs (1970), Nicholson (1974) and Schmidt (1986).

Most modern γ- and X-ray spectrometers make use of a small computer to control the measurement and store the spectrum. The advantage of such a system is that it allows us to do various data-analysis calculations during and after the measurement. During the measurement we can monitor the progress by computing the positions and areas of the critical peaks and thereby ascertain what nuclides are present as well as the rate of accumulation of counts. Many of these systems have sophisticated graphics and flexible display controls.

2.2.1 Detector bias supplies

In order to collect the charge formed in the detector, a bias voltage must be placed across the detector. The optimum bias voltage is generally specified by the detector manufacturer and may be from a few hundred volts for a small detector to over 4000 V for a large one. This voltage is chosen low enough to avoid breakdown or arcing, but otherwise as high as possible since the charge collection improves with increasing voltage. The bias voltage must be stable in order to maintain the same voltage gradients in the detector and thereby the same charge collection characteristics.

Since the voltage must not be left across the detector when it is warm, it is common practice to have some type of system that turns off the bias voltage, or sounds an alarm, when either the level of the liquid nitrogen coolant becomes low, or the detector temperatures begins to rise.

2.2.2 Preamplifiers

With a modern semiconductor-detector system a charge-sensitive preamplifier is used, and it comes as an integral part of the detector assembly. In order to minimize the electronic noise, the input stage of the preampli-

Fig. 2.8. Photograph of a Ge detector assembly showing the preamplifier components (by courtesy of Canberra Industries).
inhibited until after the pulse initiating the reset is processed. The advantage of the resistive-feedback system is that there are no reset pulses to deal with, and the advantage of the optical-feedback system is better resolution due to a reduction in the low-frequency noise because of the absence of the feedback resistor.

The height, or amplitude, of the pulse from the preamplifier should be proportional to the amount of charge collected in the detector, and if all the photon energy was absorbed in the detector, it should be proportional to this energy.

2.2.3 Amplifiers

For basic discussions of the design of amplifiers for spectrometry with semiconductor detectors, see the series of articles of Fairstein and Hahn (1965a, 1965b, 1965c, 1966a, 1966b) and the tutorial article of Goulding and Landis (1982). The important characteristics of these amplifiers are the linearity, the output pulse shape, the gain stability and the noise level. For modern systems the maximum output pulse amplitude is from 7 to 10 volts. Most amplifiers are provided with both a unipolar output (i.e., the peak part of the signal is all positive or all negative) and a bipolar output (i.e., the signal has both a positive and a negative component). To achieve optimum signal-to-noise ratio, one usually selects the unipolar output of the amplifier.

One amplifier control that the user must consciously select is the shaping time constant that determines the pulse width. Commercial amplifiers generally have several time constants for this pulse shaping network, and they may vary from 2 to 10 μs. The best resolution for the peaks in a spectrum will usually be obtained with the longer time constants, since the system can then average the noise over a longer time. This is particularly true for systems with preamplifiers with pulsed-optical feedback or with smaller feedback resistors. However, the longer time constants also lead to more random summing (see discussion in section 4.6). Therefore, one may wish to use the shorter time constants, if the system is to be operated at count rates of even 2000 s⁻¹. In most cases the analog-to-digital converter (ADC) in the multichannel analyzer will process the output pulses with any of these time constants, but care should be taken to check for proper operation if the shortest or longest time constants are selected. The lack of compatibility may be manifested in excessive nonlinearity.

Without further circuitry, the unipolar output pulse has an approximately symmetric shape with a negative undershoot and a long recovery time as shown in fig. 2.10a. At very low count rates this pulse will most often return to zero before the next pulse arrives, so the later pulse will not be affected. However, as the count rate increases many of the following pulses will have their measured amplitudes reduced because they fall on this negative tail. Since the amount of the reduction will vary with the time of arrival, the detector resolution will be degraded.

This problem has been cured by what is called “pole-zero cancelled differentiation”, first proposed by Nowlin and Blankenship (1965). This addition to the amplifier circuitry reduces the length of the undershoot as shown in fig. 2.10b and allows the system to operate at moderate count rates without any loss of resolution. If the adjustment overcompensates, the pulses have long positive tails, as shown in fig. 2.10c, giving the same
problem as with a lack of compensation. This cancellation, done by adjustments in the amplifier, must be accomplished with the whole detector–preamplifier–amplifier combination.

At still higher count rates, variations in the baseline can also degrade the resolution. This is illustrated in fig. 2.11 where the time scale has been compressed to show many pulses. The charging of coupling capacitors in AC-coupled amplifiers can produce this random-type variation in the baseline. This problem is eliminated by DC baseline restoration circuitry. Such circuits are described by Robinson (1961), Chase and Poulo (1967), and Gere and Miller (1967).

Pole-zero cancellation and base-line restoration are generally available in commercial spectrometry amplifiers. The associated literature often indicates the resolution to be expected with incident count rates of up to $10^5$ s$^{-1}$ or even higher.

The gain stability of the amplifier is very important. If a peak at channel 4000 has a width of 4 channels, a change in the gain of 0.01% or 0.4 channels in the position of the stored pulse can be significant. Not only would such a change cause a peak to be widened, but it could also distort the shape of the peak. Such a distortion could cause problems for many data-analysis routines. Since some measurements may have a duration of a day or longer, the stability should be better than 0.01% over a few days.

The influence of temperature changes on the amplifier gain, as well as the operation of all other components, must be considered. The amplifier
should have the minimum possible drift with temperature unless the temperature of its environment can be closely controlled. A reasonable specification might limit gain shifts with temperature to 0.001% K\(^{-1}\).

For most modern amplifiers that are designed for use with semiconductor detectors, the noise level is low enough that it is not a significant influence on the observed detector resolution. This resolution is determined mainly by the characteristics of the detector and the preamplifier.

Some recent amplifiers use other peak shapes. Based on the ideas of Goulding et al. (1983), commercial amplifiers have been designed to provide a pulse shape that is approximately triangular. The literature suggests that this shape allows better resolution and a greater throughput.

2.2.4 Analog-to-digital converters and data storage

The basic task in photon spectrometry is the measurement of the pulse-height distribution at the amplifier output. This is accomplished by means of an analog-to-digital converter (ADC) that converts the analog output information of the amplifier into a digital quantity. The pulse-height information from the ADC needs to be stored in an array that gives the cumulative number of counts observed in each channel. This is done simply by adding one to the contents of the channel corresponding to the pulse height measured. In addition to the pulse-height spectrum, the system normally stores the count duration (live time) in one of the first channels of the spectrum. At the end of the counting time the data in these memory locations can be read out to a storage medium such as a magnetic tape. Most modern systems include a general purpose computer that is programmed to accept the ADC output, control the counting duration, display the data as it is taken, do some simple data processing, and transfer the data on request to another device.

There are two conventional designs for an ADC – the Wilkinson type (Wilkinson 1950) and the successive-approximation type. In the Wilkinson type ADC the basic step is the simultaneous start of a clock and a voltage that increases linearly with time. When the amplitude of this ramp voltage and the amplifier output pulse are the same, the clock is stopped. Alternatively, the voltage can start at the maximum of the amplifier pulse and decrease linearly, and the clock is stopped when this voltage reaches zero. In either case the number of clock pulses represents the amplitude of the detector pulse, and an event is recorded in the corresponding data-storage location or channel. The technical difficulties of this method include sensing when the ramp voltage is equal to the maximum pulse amplitude or when it is zero. A typical modern ADC for photon spectrometry has 4096 (i.e., \(2^{12}\)) or 8192 channels. The time required to analyze a pulse increases linearly with the pulse amplitude. In addition to a constant amount of overhead time to process any pulse, with a typical 100-MHz clock and one clock cycle per channel, it takes 80 \(\mu s\) to analyze a pulse to go into channel 8000.

A different ADC concept is the successive-approximation method discussed by Robinson et al. (1968) and Gobbur et al. (1977). In contrast to the Wilkinson ADC, for the successive approximation the analysis time is independent of the pulse amplitude and is generally much smaller (a few \(\mu s\)). This system generates voltages that are half way between two other voltages and then compares the pulse amplitude with these voltages. For simplicity let us assume that we have a 1024-channel analyzer, that the top edge of channel 1024 corresponds to a pulse amplitude of 10.24 V, and that the input pulse amplitude is 7.373 V. The ADC operates as follows; it first compares the input pulse amplitude to 10.24/2 = 5.12 V and determines that the input pulse is larger. It then generates a voltage of 7.68 (i.e., 5.12 + 5.12/2) V and determines that the input pulse is smaller. The circuit proceeds to increment or decrement the comparison voltage by an amount which is a factor of two smaller at each step. By proper choice of the initial voltage, each of these increments corresponds to an integer number of channels. This process must continue until the last voltage increment corresponds to 1 channel. It is clear from this process that each analysis takes the same number of steps, since the voltage increments are always the same and the last one always corresponds to 1 channel. Therefore, the analysis time is independent of the pulse amplitude. This also means that the average analysis time is independent of the spectral shape. In contrast, for the Wilkinson ADC the average analysis time will increase if the fraction of high-energy pulses increases.

The important characteristics of an ADC are the integral linearity, the differential linearity, the zero stability, and, for the Wilkinson type, the stability of the rate of rise of the ramp voltage. Of critical importance is also the precision and stability of the live-time clock that is usually a part of the ADC.

The integral linearity indicates the deviation of the actual energy-channel relation from a linear function \(E(x) = a_1 + a_2 \cdot x\), where \(E\) is the energy, \(x\) is the channel, and \(a_1\) and \(a_2\) are constants. Heath (1969) discussed the measurement of this relationship with a precision pulser. The pulser pulses can be fed directly into the ADC to avoid measuring the nonlinearity of the amplifier. Earlier it was common for this relationship to have a large variation for the first 200 channels of a 4096-channel ADC and then be quite linear over the rest of the channel range. With modern electronic systems this variation is usually not present. If it suffices to determine the linearity of the whole electronic system, measurements can now be made much more simply with a small set of calibration sources.
Although our primary concern usually may be with the integral linearity and the energy–channel relationship, we should also be aware that there may be some differential nonlinearity, that is, that there are differences in the widths of adjacent channels. This should not be a significant problem with a Wilkinson-type ADC since the ramp voltage should be smoothly increasing. Heath (1969) discusses some measurements of the channel profiles for the Wilkinson-type ADC. However, this non-linearity is important with the successive-approximation ADC. Such differences will of course produce variations in the stored counts that are beyond the statistical scatter and thus will distort the peak shapes and complicate the spectral-analysis process. The nonlinearity can be measured with a pulser that generates a uniform distribution of pulse amplitudes. Methods of correcting for this nonlinearity have been suggested (see, for example, Cottini et al. 1963, Brendle 1977b, Casoli and Maranesi 1983, Correia and Conde 1985, and Xin and Pan 1987) that involve adding a known voltage to the pulse amplitude. By using a different voltage for each pulse, the circuit can average the channel widths over several neighboring channels.

The stability of the ADC and the associated electronics is important to the quality of the results obtained. Any drift in either the zero or the ramp of the ADC will broaden and distort the peaks and reduce our ability to resolve closely spaced peaks. Even for single peaks, the distortion will make it difficult to obtain good fits to the peaks. The zero and gain stability can be measured by monitoring the position of a peak, from a photon source or a pulser, at a low and a high channel number, respectively. Heath (1969) shows some results from monitoring the zero and gain drifts of a good and a typical ADC of that time period as measured with a pulser. Much better performance should be expected now. Although we may not choose to measure these stabilities explicitly for systems that are in routine use, we should develop a method that does monitor them implicitly, although such measurements apply to the whole spectrometer rather than just the ADC. For example, we could maintain some record of what the peak width is for some specific γ-ray energies and channel locations. If the width varies with time, attempts should be made to determine the cause and to eliminate it. The results of monitoring one system is shown in fig. 2.12 for the 122- and 1408-kV peaks from $^{152}$Eu as measured with a 114-cm$^3$ intrinsic Ge detector.

The electronic system must also determine the effective duration of the measurement. Once the ADC has begun to analyze a pulse, the input to the ADC is closed, and a closely following pulse will be rejected. This means that the ADC is dead while analyzing a pulse. In order to determine the true detector event rate, one must correct for these dead-time losses; this is achieved by operating an oscillator which serves as a clock. Only when the

![Fig. 2.12. The FWHM of the 122-kV and 1408-kV peak from $^{152}$Eu observed over a period of over 3 years as an illustration of the long-term monitoring of the stability of a Ge detector system.](image)

ADC is not busy are these clock pulses stored (e.g., in the first data channel). Thus one records the “live time” of the ADC. If this time is taken as the duration of the counting interval, the dead-time losses are properly accounted for. This live-time measuring method does not correct for any pile-up losses; this problem is discussed in sections 2.2.5 and 4.6.

2.2.5 Rise-time and pile-up rejection

There are two quite different problems that can be reduced by circuitry that rejects certain pulses. The first is related to the slow rise time of some pulses due to effects in the detector, and the second is related to pulses that are closely spaced in time and would therefore “pile-up” in the amplifier. The rise time of the pulses from a detector will depend on the location of the energy deposition within the detector. In particular, if part of the energy is deposited where the voltage gradient is small there is a significant probability for trapping, and the rise time may be longer than usual. These pulses are partly responsible for the low-energy tail of a full-energy peak. A rise-time rejection circuit will eliminate some of these pulses and improve the resolution.

The measurement of spectra at high-count rates involves other problems. We then have to deal with the overlap and partial summing of two or more
pulses. In most cases of this kind, the pulse amplitude seen by the ADC will not represent that of either original pulse. Therefore, the sum pulses do not include any useful information concerning the original photon spectrum, but, instead, fill in the continuous part of the pulse-height spectrum or even lead to additional pile-up peaks. An example of a measured spectrum distorted by pile-up is given in fig. 4.29b and computed shapes for this pile-up spectrum are reported, for example, by Wielopolski and Gardner (1976).

In many cases rejection of the summed pulses is desirable in order to prevent them from distorting the shape of the observed peaks. The most frequently applied method of determining which pulses to accept and which to reject is to measure the time spacing between them (see Goulding et al. 1983). For example, we can look at the pulses in a “fast” channel. Since for this purpose we need not maintain the information concerning the pulse amplitude, these pulses can be amplified and shaped (e.g., truncated and cut-off so that they are short) to allow fast timing. The slow-channel pulses, which are thus determined to be closely spaced in time, can be rejected by turning off the ADC at the time they would reach it. This process can be used to eliminate most of the pulses that sum in the amplifier. The remaining pulses should give a spectral shape and peak resolution that are essentially that of a low-count rate measurement.

Many pile-up rejection circuits operating in this way have been described in the literature (e.g., Souček et al. 1970, Johnson and Heath 1970, Radega 1972, Goulding and Landis 1978, Bibok and Gal 1977, Andai and Jedlovszky 1983, Chalupka and Tagesen 1986), and several pile-up rejection modules are available commercially. Apparently, some of them can process count rates in excess of $10^5 \text{ s}^{-1}$.

Chrien and Sutter (1986) developed a pile-up rejection system that incorporates digital techniques for correction of pulse-shape distortions and that contains a transient waveform recorder as the principal component. High-speed computer processing of the digitized pulse-shape allows the decision whether or not a pulse is a single or a sum pulse. Further deconvolution techniques would even make the discarding of events unnecessary.

With increasing count rate the percentage of overlapping pulses may be so high that most of the input pulses are rejected. Table 2.5 shows the counts actually stored in the spectrum as a function of the input pulse rate for two rejection systems. For the INEL system conventional amplifiers and typical amplifier time constants of 2 $\mu$s were used. In this case the maximum data storage rate is about $25 000 \text{ s}^{-1}$ and decreases as the input rate goes above $75 000 \text{ s}^{-1}$. The newer system with special fast amplifiers increases these values by a factor of about 3. In either case, this loss of data storage rate may be acceptable since the resulting spectrum contains “good” data. Chalupka and Tagesen (1986) show spectra taken with and without their rejector at a total pulse rate of $10^5 \text{ s}^{-1}$; with the rejector 50% of the counts are still accepted. If the amplifiers with very short time constants are used, the ADC must be designed to handle these narrow pulses, frequently at the expense of the energy resolution. But, in measurements at these count rates one is generally willing to accept some loss of resolution in order to be able to carry out the measurement at all.

### 2.2.6 Pulses

There are several uses that can be made of pulser that generate pulses of stable and precise relative amplitudes. These pulses are injected into the preamplifier so that they provide information on the operation of the whole electronics system. To be useful, the pulser should have
- very stable amplitude or amplitudes,
- a very stable frequency, and
- an appropriate pulse shape and amplitude.

For some applications, the pulser should provide in addition
- two, or more, pulse amplitudes which are selectable, and
- a variable frequency or random pulses.

Such pulser can be used to
- measure the resolution of the electronics system and monitor it with time,
- determine the detector contribution to the resolution and monitor it,
- measure the live time of the analyzer at low count rates (see section 4.6),
- correct for random summing or pulse pile-up (see section 4.6),
- monitor the energy calibration (see section 3.5),
- measure the linearity of the system with injection into the test input of the preamplifier,
- measure the linearity of the ADC with injection directly into the ADC, and
- provide reference points in gain and zero stabilization (see section 2.2.7).

2.2.7 Gain and zero stabilization

The best way to obtain high-quality spectra is to use electronic systems that have good stability and to operate them in a temperature-controlled environment. In this case other stability control methods should not be needed. However, some measurements must be made in less ideal conditions. In some of these conditions the use of gain stabilization may be useful.

A common method of accomplishing this is to place two narrow single-channel windows on the sides of one peak. The gain of the amplifier is controlled to keep the count rates in these two channels equal (see, for example, Yamashita 1974 and Bredgden 1977a). This naturally requires that the amplifier gain control be adjustable by external electronic means. The direction of the necessary gain change follows from the imbalance in the scalers, and the magnitude of the change must be deduced from the magnitude of the deviation. To maximize the sensitivity of the gain control, it is preferable to use a peak near the high-energy end of the spectrum. In most spectra the high-energy γ-ray peaks are weak, so it may take a significant time to accumulate enough pulses in the single channels to determine the next gain adjustment. An alternative is to use a peak from a stable pulser as the monitor line. Since the pulser pulses do not produce a Compton distribution, they do not mask the lower energy peaks, and one can adjust the pulser output rate to monitor this peak in shorter time intervals.

Whatever method is used, the gain of the system will be varied by the stabilization system, and therefore the resolution of the spectrum will be poorer than in the ideal case. Since the gain changes may not produce a Gaussian distribution, the observed peaks may deviate significantly from their usual shape.

With a modern computer-based system, there are other options. This system can be used to collect many spectra of short duration. Then the gain of each spectrum can be adjusted before the spectra are added together.

This method may be superior to using a stabilizer. Other computer-based methods have been discussed by Baran et al. (1987).

In some cases it may also be desirable to monitor the zero of the measurement system with a low-energy peak from a γ ray or a pulser. Any deviation in the position of this peak requires that one adjusts the zero control of the ADC, or some other comparable parameter, so as to return the peak to its desired position.

2.3 Gamma- and X-ray sources

A vast variety of types of sources is used in γ- and X-ray spectrometry. By a "source" we mean the macroscopic amount of material that contains the atoms emitting the nuclear and atomic radiation, not just the radiation-emitting atoms themselves; that is, the carrier and matrix materials are included in what we call a source. Examples of the various types of sources are given below, but this section deals primarily with their general properties, namely, the self-attenuation, uniformity, stability, and the production of secondary radiation within the source and its holder. Calibration sources have a special status and are discussed in detail.

2.3.1 Source types

We may distinguish between two main categories of sources: those sources that contain radioactive material and thus emit radiation continuously and those that emit photons only when irradiated by external particles or photons.

Radioactive sources usually contain the radioactive atoms either in a stable carrier material of the same element or in a matrix material of other elements or compounds. A few examples of this are
- a neutron-activated cobalt foil that contains radioactive 60Co atoms in the inactive 59Co carrier;
- a standard source produced by drying an aliquot of a calibrated solution with 152Eu atoms in an inactive europium compound as carrier;
- a radiopharmaceutical containing a 99Te-60 compound in an aqueous solution;
- a duct in the effluent-air system of a nuclear reactor that has 133Xe atoms in the air; and
- a sample with 40K in a soil matrix.

There are some cases in which the radioactive atoms are not enclosed in inactive material. Such carrier- and matrix-free sources are exemplified by
- chemically purified radium sources;
A further source of background radiation is X-ray fluorescence in the shielding material. When lead is used the X-ray energies are around 80 keV (K X rays) and 12 keV (L X rays). Since for some measurements the energies of these radiations may interfere with those of the photons under study, the internal walls of the lead castle should be cladded with a material to absorb the Pb X rays, for example, with a sheet of cadmium 1 mm thick. Pb K\textsubscript{a} and K\textsubscript{b} X rays are attenuated in such a Cd layer by factors of about 20 and 8, respectively. Further cladding with a 0.2 mm copper sheet will almost completely absorb the Cd X rays and reduce the fluorescence-radiation energy to 8 keV. Choosing only one thick sheet of, say, 5-mm iron, which has the same attenuation effect as 1-mm cadmium, would be a bad decision because the Compton-scattered radiation would appreciably increase.

Radioactive impurities in the shielding material may give rise to additional background. Lead is known to contain \textsuperscript{210}Pb (46.5-keV \( \gamma \) rays) and its daughter \textsuperscript{210}Bi (\( \beta \) rays of 1161-keV maximum energy leading to bremsstrahlung). If the inner walls of the shielding are cladded as described above, the 46.5-keV \( \gamma \) rays will be strongly attenuated. However, lead may contain other radioactive impurities, especially man-made \textsuperscript{60}Co and \textsuperscript{137}Cs. In low-level measurements, it is therefore important to use commercially available low-background lead.

In experiments involving neutrons that can reach the detector, the shield should be surrounded by paraffin and cadmium to absorb them in order to reduce (n, \( \gamma \)) reactions in or near the detector. If the neutrons can penetrate the dewar, neutron reactions in the liquid nitrogen can give rise to high-energy \( \gamma \) radiation. In these cases it is advisable to provide for a shielding between the liquid nitrogen and the detector.

Further reductions in the background by active shielding and detector construction with specially selected materials are discussed in section 5.2.2. Comprehensive reviews on the optimization of shielding measures have been given, for example, by the ICRU (1972) and Crouthamel (1970), special arrangements are described, for example, by Liguori et al. (1983), Malm et al. (1984), Zimmer and Wagner (1984), Jagam et al. (1985) and Brodzinski et al. (1985).

2.5 Performance tests

The characteristics of a newly installed semiconductor-detector system should be measured and compared with those quoted by the manufacturer. As regards the detector itself, this may be done not only for operational properties like efficiency and energy resolution, but also for geometrical properties like crystal size and window thickness. Some of the properties of the electronic system may also be tested. Furthermore, several characteristic spectra should be taken and stored in order to facilitate a later judgement as to whether deviations from the initial performance have occurred.

The manufacturer's specifications of the efficiency, energy resolution, peak shape and peak-to-Compton ratio apply to the particular detector--preamplifier--amplifier system and the conditions chosen by the supplier. In order to check the detector performance against these specifications, we must conduct the measurements with a comparable system operated under comparable conditions. In particular, we must use a comparable amplifier time constant, since it plays a key role in the energy resolution observed. Time constants that are too high as well as those that are too low can deteriorate the resolution. The best resolution is usually obtained with rather long time constants. If it is intended to perform regular measurements under different conditions than those used by the manufacturer, test measurements should also be made under these conditions.

To obtain optimum performance, it is mandatory to use a modern spectroscopy amplifier and to adjust it in accordance with the instructions of the manufacturer. This applies especially to the pole-zero cancellation and the base-line restoration adjustments.

2.5.1 Efficiency

The efficiency relative to NaI, \( \epsilon_r \), can be determined by actually carrying out the NaI(Tl) detector measurement, but more often the well-established
full-energy-peak efficiency of a 7.62-cm diameter $\times$ 7.62-cm length NaI(Tl) detector for a source distance of 25 cm is used, which is $\epsilon_{\text{NaI}} = 1.2 \times 10^{-3}$.

From a measurement with a $^{60}\text{Co}$ standard source of activity $A$ positioned at a distance of 25 cm from the detector endcap, we obtain

$$\epsilon_r = \frac{N}{T \cdot A \cdot \epsilon_{\text{NaI}}} = 0.83 \cdot 10^3 \cdot \frac{N}{T \cdot A} \quad (2.10)$$

where $N$ is the number of counts in the 1332-keV peak accumulated within the measuring time $T$. This result has to be multiplied by 100 to get $\epsilon_r$ in %. The source activity should be less than 500 kBq to keep the pile-up losses to a negligible level. To achieve a statistical uncertainty of 1% at least 10,000 counts should be accumulated. For a detector with $\epsilon_r = 10\%$ and a source with $A = 100$ kBq, we will obtain this number of counts in about 1000 s.

For large n-type detectors, which are also efficient for low energies, some suppliers specify the ratio between the heights of the 22.1-keV $K_a$ X-ray peak and the 88.0 keV peak from a $^{109}\text{Cd}$ source. For a test of this ratio, the source should be at a sufficient distance for the photons to penetrate the window of the detector approximately normal, so that the path length through the window, and thus the attenuation of the X rays, is minimized.

2.5.2 Energy resolution and peak shape

The FWHM can be determined with uncalibrated sources at any source–detector distance. However, the total count rate in the spectrum should not exceed 1000 s$^{-1}$, since pulse pile-up may noticeably broaden the peaks. For electronic shaping-time constants longer than 8 $\mu$s, the count rate should be even lower. On the other hand, too low a count rate will require a long measuring time and thereby increase the risk of deterioration of the resolution due to instrumental drifts. To obtain adequate counting statistics, at least 20,000 counts should be accumulated in the peak.

The energy resolution depends on the amplifier time constant $\tau$. In order to reproduce the supplier’s specification, $\tau$ should be chosen correspondingly. Generally, the supplier will quote the resolution as measured at rather long time constants to obtain the smallest possible FWHM. In addition, one should also determine the energy resolution at shorter time constants. As long as no unacceptable increase in the FWHM is observed, the choice of a shorter time constant in the actual measurements should be considered, since pile-up effects can thus be appreciably reduced.

For measurements of the energy resolution the amplifier gain should be adjusted so that the FWHM is 4 channels or more. In a visual derivation of the FWHM, as illustrated in fig. 2.26, partial channels must be included.

An energy calibration can be provided by two peaks (energies $E_1$ and $E_2$), e.g., those originating from the nuclides for which the FWHM is usually specified, namely,

$^{60}\text{Co}$ with $E_1 = 1173.2 \text{ keV}$ and $E_2 = 1332.5 \text{ keV}$,

$^{55}\text{Fe}$ with $E_1 = 5.90 \text{ keV}$ and $E_2 = 6.49 \text{ keV}$,

$^{57}\text{Co}$ with $E_1 = 14.4 \text{ keV}$ and $E_2 = 122.1 \text{ keV}$.

Denoting the FWHM in channels by $w_c$, and in units of the energy by $w$, we get the relation

$$w = \frac{E_2 - E_1}{c(E_2) - c(E_1)} w_c, \quad (2.11)$$
2.5.3 Detector size

In addition to the operational detector properties the manufacturers supply information on the crystal dimensions. For large coaxial detectors the efficiency for $^{60}$Co relative to NaI is a measure of the crystal volume, although there is no unequivocal relation between this efficiency and the volume. Many users are satisfied when they reproduce the specified efficiency, and in these cases a determination of the crystal dimensions may be of no interest. On the other hand, there are users who need the dimensions of the sensitive volume of the detector, for example, because they wish to perform full-energy-peak efficiency calculations (see section 4.1.2). In such cases it is also important to know the distance between the crystal surface and the window, and whether or not the crystal is mounted coaxially with its housing.

An effective way to obtain information on the dimensions and location of the crystal is to take X-ray photographs. In fig. 2.28 the image of a planar high-purity germanium detector is shown (Johnston 1985). At least two photographs of this type taken from different directions are needed to determine the detector position in the housing, but the displacement of this crystal from the axis of the housing can be clearly seen in this particular

with $e(E)$ being the channel corresponding to the energy $E$. Equation (2.11) applies correspondingly to the determination of the FWIM (see fig. 2.26) and the FWFM. For coaxial detectors the peak-to-Compton ratio $P/C$ is a further specification. It is obtained from a pulse-height spectrum recorded with a $^{60}$Co source as illustrated in fig. 2.27.

As a part of the resolution tests, it is also advisable to connect a stable pulse generator to the test input of the preamplifier and to measure the FWHM of the pulser peak in the spectrum. Assuming that the pulser amplitude remains stable during the measurement, the pulser-peak width $w_p$ is due only to the electronics. Knowledge of the initial test values of both $w$ and $w_p$ may help in distinguishing to what extent any subsequent deterioration in resolution occurred in the detector and/or the electronics.

Due to the difference in the shapes of the pulser and detector pulses, an optimum adjustment of the amplifier pole-zero cancellation is not always simultaneously possible for both types of pulses. Proper adjustment for detector pulses usually leads to undershoots for pulser pulses, and the presence of these pulses may cause deterioration of the photon-peak shapes. The FWHM, FWIM and FWFM should therefore always be measured with the pulse generator off.

Timing capabilities are of no interest to users merely taking pulse-height spectra and determining emission rates or activities. Readers interested in procedures for checking the timing characteristics are referred to standards published by ANSI/IEEE (1986) and IEC (1973).
example. Proof that the crystal is circular would require another photograph taken from the front side.

An alternative method, by which the size of the sensitive crystal volume is obtained, is to scan the crystal in various directions with a well-collimated beam of photons. Figures 2.29 and 2.30 show examples of scans across, and normal to, the front surface of a planar and a true-coaxial germanium crystal. In this case a small spherical $^{241}\text{Am}$ source (1 GBq) was placed at the entrance of a lead collimator 20-mm long with a hole 1 mm in diameter. The source–collimator assembly was moved in 1-mm steps and the counts in the 59.5-keV peak were registered. The position, diameter and thickness of the sensitive volume can thus be determined with a resolution of about 1 mm. Several scans, across different diameters or parallel to one another, are needed to determine the center of the crystal and to ensure that the crystal is circular. The diameter of the insensitive core of the true-coaxial crystal was measured in the same way (see fig. 2.30).

Usually any structure in the surface and other deviations from the cylindrical shape can not be found by this method because the response of the detector to the parallel beam is independent of the source-to-detector-surface distance. The energy of the photons used for the scanning should be high enough to ensure penetration of window, detector housing and crystal holder. On the other hand, it should be low enough to keep the collimation effective. The 59.5-keV photons from $^{241}\text{Am}$ are usually an excellent choice because their energy is high enough to penetrate housing and crystal-holder materials as well as insensitive germanium layers, and because their mean penetration depth into germanium (about 1 mm) is low enough to gain information on variations in the thickness of insensitive surface layers. A detailed description of a scanning device and many scans have been given by Hansen et al. (1973). Campbell et al. (1971) used an interesting $\text{NaI(Tl)}-\text{Ge(Li)}$ coincidence arrangement to take advantage of the $180^\circ$ relationship between two annihilation quanta to achieve collimation.

### 2.5.4 Windows and dead layers

The thickness of the material in front of the sensitive crystal volume cannot be checked easily. The shape of the efficiency curve in the low-energy region provides the main information from which the thickness of these materials may be estimated. For planar detectors an overall check may be made by calculating the attenuation in the detector window, the

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Fig. 2.29. Scans (a) across, and (b) normal to, the front surface of a planar, circular germanium crystal (diameter: 25 mm; thickness: 18 mm) (from Debertin and Grosserndt 1982).
crystal contact layer and the germanium or silicon dead layer from the specified thicknesses and comparing the result with the shape of the measured efficiency curve (full-energy plus Ge- or Si-escape peak efficiency). In most cases it will not be possible to use the differences to adjust the various thicknesses in a unique way, but an approximate agreement should be sufficient to indicate that the specified thicknesses are reasonably accurate. We will return to this method in the discussion of the efficiency calibration at low energies (section 4.2.2).

The thickness of a gold contact layer can be obtained by exciting the gold atoms with photons of an energy greater than the gold L-absorption edge and measuring the Au L\textsubscript{\textalpha} X rays as described by Shima et al. (1980) and Maenhaut and Raedonck (1984).

A clever method (Forcinal 1973, Pessara 1983) for determining the thickness of a germanium dead layer takes advantage of the fact that the mass attenuation coefficient of germanium changes from $\mu/\rho = 27 \text{ cm}^2 \text{ g}^{-1}$ below the K edge at 11.1 keV to 209 cm$^2$ g$^{-1}$ above it. A source like $^{75}$Se that emits As X rays with the K\textsubscript{\textalpha} lines at 10.5 keV slightly below and the K\textsubscript{\textbeta} lines at 11.7 keV slightly above the Ge-K edge, is useful for this measurement. If we assume that the efficiency of a detector without a dead layer does not change in this small interval, the ratio of the K\textsubscript{\textalpha} full-energy-peak counts, $N_{\alpha}$, to the K\textsubscript{\textbeta} full-energy plus escape-peak counts, $N_{\beta}$, will be equal to the ratio of the X-ray-emission probabilities $p_{\alpha}$ and $p_{\beta}$:

$$N_{\alpha}/N_{\beta} = p_{\alpha}/p_{\beta}. \quad (2.12)$$

With a germanium dead layer of thickness $t$, we obtain

$$N_{\alpha}/N_{\beta} = \frac{p_{\alpha} e^{-\mu_{\alpha} t}}{p_{\beta} e^{-\mu_{\beta} t}}. \quad (2.13)$$

With

$$p_{\alpha} = 0.498,$$

$$p_{\beta} = 0.076,$$

$$\mu_{\alpha}/\rho = 32.5 \text{ cm}^2 \text{ g}^{-1},$$

$$\mu_{\beta}/\rho = 170 \text{ cm}^2 \text{ g}^{-1},$$

$$\rho = 5.323 \text{ g cm}^{-3}$$

For Fig. 2.30. Scans (a) across, and (b) normal to, the front surface of a true coaxial, circular germanium crystal (diameter: 32 mm; thickness 49 mm) (from Debertin and Grodewegt 1982).
we get 
\[ N_a/N_B = 6.55 \times e^{0.073 \cdot t} \quad (t \text{ in } \mu\text{m}). \] (2.14)

Because of the limited accuracy of \( p_a \) and \( p_B \), dead layers of less than 0.5 \( \mu\text{m} \) cannot be determined in this way. However, if the same source is also measured with a Si(Li) detector for which eq. (2.12) should be valid, \( p_a/p_B \) in eq. (2.13) can be replaced by the ratio of the full-energy-peak counts from a Si(Li) detector. Pessara (1983) has shown that the thickness of a dead layer of 0.3 \( \mu\text{m} \) can be determined by this method with an uncertainty of 15%.

Baker et al. (1987) determined the Be-window and Si-dead-layer thickness by making measurements at several energies, above and below the Si K edge, with well-collimated X-ray beams, incident both normal to the detector surface and at an angle (38.5°) to the normal.

The problems related to the determination of the thicknesses of each of the various attenuating layers have been discussed comprehensively by Campbell et al. (1985) and Campbell and McGhee (1986). These authors include incomplete charge-collection effects in their considerations.

### 2.5.5 Background spectrum

When a decision has been made on a definite measuring geometry, a background spectrum, preferably measured for a period of a few days, should be taken, plotted, evaluated, and the results recorded. A typical spectrum for an unshielded detector is shown in fig. 2.31. Most of the peaks can be identified as being from the Ra and Th decay chains; their energies and the peak count rates are given in table 2.9. The effect of shielding the whole detector assembly, including the dewar, by a 5-cm-thick lead castle is seen by comparing columns (a) and (b) of the table. An interesting feature is the disclosure of additional peaks in the latter spectrum, for example, the 185.7-keV peak due to \( ^{235}\text{U} \) which is masked under the 186.2-keV peak of \( ^{226}\text{Ra} \) in the spectrum taken without shielding. These \( \gamma \) rays are evidently not attenuated by the lead, so they must originate in the detector assembly, probably from traces of uranium in the aluminum of the detector housing (see section 5.3.1 for a further discussion of radionuclidic impurities in the detector assembly).

The total background count rate above a certain energy should be recorded. For the measurements referred to above, these count rates were 280 s\(^{-1}\) without and 4 s\(^{-1}\) with shielding (discriminator at 20 keV). Any increase in this rate at a later time may suggest that the detector assembly is contaminated, that other sources were placed in the neighborhood of the

### Table 2.9

<table>
<thead>
<tr>
<th>( E ) (keV)</th>
<th>Origin of photons</th>
<th>Count rate (10(^{-3}) s(^{-1}))</th>
</tr>
</thead>
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Some low-energy peaks may be due to resonance fluorescence in the materials surrounding the crystal. In the above example Pb X rays from the detector or that direct or scattered radiation from a nearby nuclear facility has increased.

Fig. 2.31. Pulse-height spectrum of the natural background obtained with an n-type high-purity germanium detector (efficiency relative to NaI: 25%). The detector was unshielded. Energies given in keV.
nearby shielding and Ba X rays from the concrete of the room walls are observed. This must be borne in mind in actual measurements where the photons from the source may produce a fluorescence radiation "background". For example, when sources are measured in glass ampoules, Ba X-ray peaks may be observed, since some types of glass contain barium.

2.5.6 Routine performance checks

In the course of the operation of a semiconductor-detector system, regular checks of the system properties should be performed. The frequency of these checks will depend on the required accuracy and reliability of the measurements and may be carried out daily, weekly or monthly. In any case, they are necessary after any detector warm-up period, repairs, power failure, readjustment, replacement of parts of the electronics, or a change of the amplifier time constant.

The energy resolution and the stability of the energy and efficiency calibration can be checked in one step by taking a pulse-height spectrum of a source emitting photons of several energies distributed over the energy range of interest. For an energy range up to 1500 keV, a $^{152}$Eu source is a good choice. $^{152}$Eu emits X rays at 40 and 46 keV and $\gamma$ rays in the range from 122 to 1528 keV with main lines at 122, 245, 344, 779, 964, 1112 and 1408 keV. For the low-energy range, $^{55}$Co (energies at 6.4/7.1, 14.4, 122 and 136 keV) or $^{241}$Am (useful energies at 11.9, 13.9, 26.4 and 59.5 keV) may be used.

Each time a check measurement is performed, a plot of the spectrum should be made and the main full-energy peaks analyzed with the program routinely used. Peak positions, areas (corrected for decay) and widths should be recorded on a control chart or data file and compared with the results of the previous check runs. As well as keeping a record of the results from the check measurements, it may be advantageous to preserve the spectra. If, at a later date, the analysis program is changed, these spectra can be reanalyzed to determine the difference between the programs in order to maintain long-term stability records. Since in all performance checks relative values at a given energy are compared, even for the efficiency check, the source need not be calibrated, and coincidence-summing corrections need not be considered. For efficiency checks it is important that the source position is well reproducible. Figure 2.32 is an example of
the results of routine efficiency checks with a $^{152}$Eu source over a period of seven years. It is interesting to note that the efficiency remained approximately constant at 122 keV, but decreased at 1408 keV within the first three years by about 1%, remained constant for three years and then decreased again.

If the first spectrum of the check source has been taken immediately after the initial energy and efficiency calibration and if no significant changes in the later check measurements are observed, in principle, no repetition of the efficiency calibration procedure is necessary. To be sure, however, we recommend repeating the calibration semiannually with the proper sources. A further routine procedure should be a daily check of the total background count rate. If any changes are observed a background spectrum should be taken and compared with the spectrum of the original performance test.

Changes of the experimental setup in the surroundings of the source or the detector may lead to a change in the region of the backscatter peak (see section 3.1.1). It is therefore worth taking a spectrum of, for example, a $^{60}$Co or $^{137}$Cs source from time to time and to check whether the spectrum shape in this region has changed.

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### Spectrum analysis and energy measurements

The usual objective of photon measurements with semiconductor detectors is the determination of the number and energy of photons being emitted by a source. In many applications this information is used to identify the radionuclides present in the source and to determine the activities of the individual components. In research measurements the quantities of interest may be the photon energies themselves or the relative emission rates of the various groups of photons.

The task in gamma- and X-ray spectrometry is then the analysis of the peaks in pulse-height spectra that correspond to full-energy absorption events. The peak location is a measure of the photon energy and the peak

![Flow chart for typical \(\gamma\)-ray spectrum analysis program.](image-url)
area of the photon emission rate. For energy measurements the pulse-height scale must be calibrated with sources emitting photons of known energies.

In order to compute an emission rate \( R \), the source–detector system must be calibrated with respect to its full-energy-peak efficiency \( \epsilon \).

In the subsequent sections we will discuss
- the shapes of spectra and peaks in section 3.1;
- procedures for automatically determining the peak location in section 3.2;
- methods to obtain the peak centroid and area in section 3.3;
- details of the energy calibration in section 3.4; and
- routine and precise energy measurements in section 3.5.

The efficiency calibration and emission-rate determinations are described in chapter 4. The sequence of operations in the analysis of the peaks in a spectrum is summarized in fig. 3.1.

3.1 The shape of spectra and peaks

The photon spectrum of a source usually consists of discrete lines of very small width, while the measured pulse-height spectrum is a continuous distribution due to diverse effects described in section 1.4. The full-energy peaks (or total-absorption peaks) in this spectrum may only amount to a small fraction of the total counts, but they provide the useful information. The rest has to be considered as spectral background, unwanted but unavoidable. After the discussion of the general structure of pulse-height spectra produced by photons in semiconductor detectors in section 3.1.1, we will consider analytical functions that represent the shapes of the full-energy peaks in sections 3.1.2 and 3.1.3.

A typical full-energy peak due to \( \gamma \) rays of \(^{60}\)Co is illustrated in fig. 3.9. It becomes evident from fig. 3.9 that it is advantageous to include two functions in this representation, one for the background in the peak region and one for the peak itself. The discussion will be mainly in terms of \( \gamma \)-ray spectra; special aspects of X-ray spectra will be considered in section 3.3.4.

3.1.1 The shape of spectra

Comprehensive collections of experimental pulse-height spectra for about 200 radionuclides have been published by Heath (1974) and Adams and Dams (1970). As examples, two simple spectra, one for \(^{137}\)Cs and the other for \(^{88}\)Y, are shown in figs. 3.2 and 3.3.
Spectrum analysis and energy measurements

Fig. 3.4. Experimental pulse-height spectrum of $^{37}$S and calculated spectrum components (from Gardner et al. 1986): (1) flat continuum; (2) exponential tail of the full-energy peak; (3) full-energy peak; (4) Compton-electron scattering continuum; (5) continuum between 4 and 3; (6) single-escape peak; (7) double-escape peak; (8) continuum between 6 and 7.

Several attempts have been made to calculate the shape of spectra either by Monte Carlo simulation (e.g., Gardner et al. 1986) or by using semi-empirical models (e.g., Jin et al. 1986). In fig. 3.4 various calculated spectrum components are depicted for 3103-keV γ rays. The contributions to the pulse-height spectrum are due mainly to interactions by photoelectric absorption, Compton scattering and pair production suffered by the primary photons that reach the detector directly. Details on these effects and on the energy and atomic-number dependence of the photon attenuation in matter have been discussed in section 1.4.

Photoelectric absorption in the crystal is expected to yield a pulse corresponding to the full energy of the photon (peak 3 in fig. 3.4), if three conditions are fulfilled:

- First, Ge or Si X rays, originating from the rearrangement of the atomic-shell electrons after emission of the photoelectron, have to be absorbed in the crystal. If they escape the event contributes to one of the X-ray escape peaks below the full-energy peak.

- Second, the photoelectron must lose its whole energy within the sensitive volume of the crystal. Bremsstrahlung losses and escaping photoelectrons give rise to a pulse continuum from zero to full energy (part of component 1 in fig. 3.4).

- Third, trapping effects and charge-collection losses have to be negligible. If they are not, the event will contribute to the low-energy tailing of the peak (component 2 in fig. 3.4). Whether or not it is counted as a full-energy-peak event depends on the peak-analysis method.

X-ray escape plays a significant role for germanium detectors at photon energies below 50 keV, but it is less important for silicon detectors where it amounts to less than 1% for energies higher than 5 keV. Figure 3.5a shows the pulse-height distribution obtained with a planar Ge detector for the X rays emitted in the decay of $^{85}$Sr. Figure 3.5b is a spectrum taken with a Si(Li) detector and the same source. Since both $K_\alpha$ and $K_\beta$ X rays can escape, we get an escape-peak doublet for germanium 9.9 keV and 11.0 keV below the full-energy peak. The Si K X rays have energies of 1.7 keV and 1.8 keV, so the escape peaks are not resolved by the detector. The ratio of the escape-peak and full-energy-peak areas as a function of energy is discussed in section 4.2.2.

The effect of charge-collection losses, which lead to a tailing on the low-energy side of the full-energy peak, is particularly pronounced in Si(Li)-detector spectra for photon energies just above the Si K edge. Inagaki et al. (1987) and Geretschläger (1987) have shown that up to one third of the full-energy-absorption events may be shifted down into a shoulder-type tail distribution ranging down to half the photon energy.

While the photoelectric effect dominates at low energies, the Compton effect is the most frequent process in the energy range from 150 keV to 9 MeV for germanium and from 50 keV to 15 MeV for silicon. The Compton electrons, whose energy is absorbed in the detector, give rise to a continuous distribution extending from zero energy to $E/(1 + m_{\gamma e}c^2/2E)$ (see eq. (1.15)), where $E$ is the primary photon energy and $m_{\gamma e}c^2$ the electron rest energy. Typical Compton distributions are shown in figs. 3.2, 3.3 and 3.4 (component 4). Because of the limited detector resolution, the sharp Compton edge of the theoretical distribution (see fig 1.21) is smeared out in the pulse-height spectrum, and the maximum count is slightly below the calculated energy for the edge. The scattered photon, with an energy between $E/(1 + 2E/m_{\gamma e}c^2)$ and $E$, can again interact in the crystal. If it interacts by the photoelectric effect, the sum pulse (Compton electron plus photoelectron) contributes to the full-energy peak. In the case that the scattered photon interacts by a further Compton effect with the second scattered photon escaping from the crystal, the pulse appears anywhere in the continuum below the peak (component 5 in fig. 3.4). It is these multiple Compton events which give rise to deviations of the observed pulse-height spectrum from the theoretical one-event distribution.
Pair production starts to play a role for energies above 1.5 MeV although it is energetically possible from \( 2m_e c^2 = 1.022 \) MeV upwards. Full absorption of the kinetic energy of the electron–positron pair results in the

Fig. 3.6. Type of photon interactions in the detector surroundings; \( \gamma \) : emitted \( \gamma \) rays, \( \gamma' \) : Compton-scattered \( \gamma \) ray, \( \gamma_\text{a} \) : annihilation quantum following pair production, \( \gamma_\text{x} \) : X ray following photoelectric absorption.

Fig. 3.7. Pulse-height spectrum of a \(^{55}\text{Fe}\) source deposited on a steel support. Detector: Si(Li), 3-mm thick.
“double-escape” peak at \( E - 2m_ee^2 \) if both positron-annihilation quanta escape. If one of them interacts in the crystal the sum pulse either contributes to the single-escape peak at \( E - m_ee^2 \), or to the distribution between \( E - 2m_ee^2 \) and \( E - m_ee^2 \). Interaction of both quanta can lead to a sum pulse corresponding to the full energy or to a pulse in the continuum between \( E - 2m_ee^2 \) and \( E \). The spectra in figs. 3.3 and 3.4 (components 6 to 8) reflect the characteristic features of pair production.

The photons emitted from the source can also interact with the material surrounding the crystal as illustrated in fig. 3.6. The resulting secondary photons, that is, X rays, Compton-scattered and annihilation quanta, may reach the crystal and so add to the pulse-height spectrum. We will consider the three effects in turn.

The photoelectric effect results in excited atoms which emit characteristic X rays. Therefore, we may observe in the spectrum, for example, K and/or L X rays from a lead shielding or collimator, from a gold contact layer on the crystal, from a steel support of a source, or from the elements of the material containing the radioactive substance. Figure 3.7 shows the pulse-height spectrum obtained with a \(^{58}\)Fe source on a steel support. The energy of the Mn K X rays emitted by the source is not high enough to excite a K electron in iron, but K X rays of low-Z components (Cr, V) of the steel, as well as of the argon in the surrounding air and of the chlorine in the FeCl\(_3\) of the source, are observed.

Compton-scattered photons from the surrounding material have energies between \( E/(1 + 2E/m_ee^2) \) and \( E \), depending on the scattering angle. Photons scattered into backward angles usually predominate and lead to the backscatter peak near the lower end of the energy range. Examples are given in figs. 3.2 and 3.3. For low primary photon energies this scattering distribution is very near the full-energy peak and may even not be resolvable. Not surprisingly, the percentage of pulses due to scattered secondary photons is particularly high for matrix sources like aqueous solutions. This is illustrated by fig. 3.8 where spectra of \(^{60}\)Co obtained with a point and a volume source are compared.

For high-energy photons, annihilation quanta following pair production in the surrounding material give rise to a peak at 511 keV. Contributions to this peak may also be due to annihilation of positrons emitted in \( \beta^+ \) decay of the radionuclide under study.

There are also other effects which may cause deviations of the pulse-height spectrum from the expected shape. Beta particles and conversion electrons, when reaching the crystal in case the detector assembly has a very thin window, and bremsstrahlung may augment the continuum distribution. If a radionuclide decays via a photon cascade, two or more photons may be detected simultaneously thus leading to a summing distribution with a peak at a position corresponding to the sum of the photon energies (see section 4.5). Apart from these real coincidences, random summing, in particular at high count rates, results in peak and spectrum distortion (see section 4.6). “Ghost” peaks due to defective or unsatisfactorily adjusted electronics may also occur but they can usually be identified by their abnormal shape and width.

### 3.1.2 Shape of the spectral background

As stated in the introduction to section 3.1, it is advantageous to describe the data in the region of a peak by two analytical functions – the first to represent the “background” and the second to represent the “peak”. It should be emphasized that we wish to define “background” in an arbitrary way. The most basic definition of “background” might be the spectrum observed with no source; that is, the spectrum from any radiation originating outside the source. This we will call the room or environmental background. When discussing \( \gamma \) rays of one particular energy in a spectrum it might be reasonable to define the “background” as the spectrum that would be observed if all the radiations, except the \( \gamma \) rays with the energy of interest, were present. This would include the effect of the higher energy \( \gamma \) rays as well as the environmental background. However, in the spectral analysis, it is customary to include even more in the term “background”; namely, we wish to include everything that is not part of the “peak”. In fig.
3.9 the increase in the height of the spectrum from the flat portion above the peak to the flat portion below the peak is produced by events that would be in the full-energy peak, but are recorded below it because of the escape of primary or secondary electrons from the sensitive volume of the detector. We define this step-like increase as part of the background rather than part of the peak.

A large number of analytical functions have been used to represent this spectral background. These functions are often made up of two parts—first, a low-order polynomial for the contribution that originates from higher energy photons and underlies the whole peak region, and second, a function to represent the step-like increase on the low-energy side of the peak. The expressions suggested for the first part vary from a constant to a third-order polynomial in the channel number. Kokta (1973) and Hertogen et al. (1974) have discussed these expressions and the number and location of the channels to use to determine the coefficients of the quadratic and cubic terms. Hertogen et al. (1974) talk of using 30 channels on each side of the centroid in this determination; but, this large number of background channels is usually not available. Less extensive discussions of these background functions are given by Quittner (1969) and Laitano et al. (1979). Generally, a linear function approximates the background sufficiently well unless there is a Compton edge in the region. Quadratic or cubic terms may cause the background function to follow random fluctuations in the peak-channel counts or some high-side tailing, thereby creating an unrealistic background shape. This is especially true if the number of channels in the background region is small.

Several of the functions that have been proposed to represent the step-like increase of the background are given in table 3.1 and illustrated in
Spectrum analysis and energy measurements

### Table 3.1

Step-like background functions suggested in the literature (from Helmer and Lee 1980).

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<th>Number</th>
<th>Reference</th>
<th>Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>B1</td>
<td></td>
<td>Step ( f(x) = \begin{cases} 1 &amp; \text{for } x &lt; X \ 0 &amp; \text{for } x &gt; X \end{cases} )</td>
</tr>
<tr>
<td>B2</td>
<td>Sanders and Holm (1969)</td>
<td>( 1 - e^{x-B} )</td>
</tr>
<tr>
<td>B3</td>
<td>Robinson (1970)</td>
<td>( \frac{1}{2} \left[ 1 + \frac{1}{\sigma} \arctan \left( \frac{X - P_2 x - X}{P_1 \sigma} \right) \right] )</td>
</tr>
<tr>
<td>B4</td>
<td>Kern (1970)</td>
<td>( 1 - \left[ 1 + \left( \frac{x - X}{\sigma} \right)^2 \right]^{-1/2} )</td>
</tr>
<tr>
<td>B5</td>
<td>Teoh (1973)</td>
<td>( 1 + e^{(x-x)/0.75w} )</td>
</tr>
<tr>
<td>B6</td>
<td>Phillips and Markow (1976)</td>
<td>( \frac{1}{2} \text{erfc}(x-X)/2^{1/2}a )</td>
</tr>
<tr>
<td>B7</td>
<td>Sasamoto et al. (1975)</td>
<td>( \frac{1}{2} \left( 1 - e^{2x-x-X}/\sigma \right) ) for ( x &lt; X )</td>
</tr>
<tr>
<td>B8</td>
<td>Gunnink (1979)</td>
<td>( 1 - \sum_{i=x}^{\infty} y_i / \sum_{i=0}^{\infty} y_i )</td>
</tr>
</tbody>
</table>

**Symbols:**
- \( x \) = channel number (or independent variable),
- \( y_i \) = net counts in channel \( i \),
- \( X \) = center of the peak (in channels),
- \( w \) = FWHM
- \( \sigma \) = Gaussian width parameter, \( w = (8 \ln 2)^{1/2} \sigma \),
- \( P_1, P_2 \) = parameters to be determined from fit to experimental data and
- \( \text{erfc} \) = complementary error function.

Some of these functions are related to the way the increase in the background is believed to occur. The simplest ideas suggest that, neglecting the broadening due to the detector resolution, this distribution is flat and extends to the centroid of the peak. Therefore, one might use the step-function, B1 in the table. However, more of the physics of the process can be simulated. We would expect the discontinuity of the step to be broadened in the same manner as the monoenergetic \( \gamma \)-ray line is broadened; that is, the step should be convoluted with a Gaussian whose width is that of the main peak. This convolution produces the complementary error function, B6.

The functions B2 and B4 go to zero at the center of the peak. As indicated in the previous paragraph, this does not represent the physics of the situation. Among the continuous functions that do not go to zero at the centroid (i.e., B3, B5, B6, and B7), there are two notable differences. First, the arctan function, B3, approaches the asymptotic values of 0.0 and 1.0 much more slowly than the other three functions. Second, the slopes of the functions at \( x = 0 \) are different. However, the latter difference is not inherent, since by changing the slope determining parameters of B5 and B7, all of these slopes can be made nearly equal (see fig. 3 of Helmer and Lee 1980).

The function B8 is not included in fig. 3.10 since it depends on the experimental data that make up the particular peak. This function is interesting for two reasons. First, it is the function that one obtains if a step function is broadened by the experimental peak shape. Therefore, it is the experimental equivalent of the complementary error function B6 and, in principle, might be the best shape. Second, the function is computationally simple, so it is much faster to compute than the error functions, and this was considered an advantage for analysis programs on computers of limited speed. However, this function does have one distinct disadvantage. Since it depends on the data of a particular peak, it must be computed separately for each peak. Therefore, it can not be computed and normalized as part of an analytical peak-shape function.

We would conclude these comments with the suggestion that the best analytical representation of the background probably comes from expression B6, or one of the approximations to it, that is, B1 and B8. At the same time it should be noted that there is little practical difference between any functions that approximate a step function. This is due to the fact that the differences between them are largest near the peak centroid where their contribution is negligible compared to the Gaussian peak component.

There is another method of defining the spectral background which does not rely on an analytical representation. This involves the approximation of the background by a set of smoothed and interpolated points. A method of generating such a background spectrum is to do an iterative smoothing of the data until the peaks disappear. Methods of generating this smoothed spectrum have been discussed by Ralston and Wilcox (1969), Grosswendt (1971), Gunnink and Niday (1972), Westmeier (1981), Burgess and Tervo (1983) and Tervo et al. (1983). Burgess (1984) has compared some of these specific methods. This representation of the background should include the step-like portions. Given this background spectrum, the peaks can be analyzed by actually, or effectively, subtracting this spectrum. The proper peak-shape function will, of course, depend on the extent to which the method includes the tailing in the background. If one is involved in an application in which areas of small peaks are important, care will be necessary to prevent the smoothing process from including any small peaks as part of the spectral background.
Table 3.2
Analytical forms of peak-shape functions assuming no high-energy tailing (from Helmer and Lee 1980).

<table>
<thead>
<tr>
<th>Number</th>
<th>Reference</th>
<th>Program name</th>
<th>Main portion</th>
<th>Function</th>
<th>Additive tail</th>
</tr>
</thead>
<tbody>
<tr>
<td>S1</td>
<td>Many</td>
<td></td>
<td>Gaussian = $Y e^{-(x-x)^2/2w^2}$</td>
<td>None</td>
<td></td>
</tr>
<tr>
<td>S2</td>
<td>Routti and Prusia (1969)</td>
<td>SAMPO</td>
<td>$e^{-(x-x)^2/w^2}$ for $x &gt; X - J$</td>
<td>$P_e^{p}e^{-(x-x)^2/2w^2}(1 - e^{p}(x-x)^2/2w^2)$ for $x &lt; X$</td>
<td>None</td>
</tr>
<tr>
<td>S3</td>
<td>Sanders and Holm (1969)</td>
<td>GAMANAL</td>
<td>Gaussian</td>
<td>$P_e^{p}e^{-(x-x)^2/2w^2}$ for $x &lt; X$</td>
<td>None</td>
</tr>
<tr>
<td>S4</td>
<td>Seybold and Niday (1972)</td>
<td></td>
<td>Gaussian</td>
<td>$P_e^{p}e^{-(x-x)^2/2w^2}$ for $x &lt; X$</td>
<td></td>
</tr>
<tr>
<td>S5</td>
<td>Kern (1970)</td>
<td></td>
<td>Gaussian</td>
<td>$P_e^{p}e^{-(x-x)^2/2w^2}$ for $x &lt; X$</td>
<td></td>
</tr>
<tr>
<td>S6</td>
<td>Hooet (1971)</td>
<td></td>
<td>Gaussian</td>
<td>$P_e^{p}e^{-(x-x)^2/2w^2}$ for $x &lt; X$</td>
<td></td>
</tr>
<tr>
<td>S7</td>
<td>Baba et al. (1973)</td>
<td></td>
<td>Asymmetric Gaussian</td>
<td>$e^{-(x-x)^2/2w_1^2}$ for $x &gt; X$</td>
<td></td>
</tr>
<tr>
<td>S8</td>
<td>Schick (1974)</td>
<td>SKEWGAUSS</td>
<td>Same as S2</td>
<td>$e^{(2z - 2z^2)/2z^2}P_1(x - X + J)^n$ with $n = 4$ suggested</td>
<td></td>
</tr>
<tr>
<td>S9</td>
<td>Phillips and Marlow (1976)</td>
<td>HYPERMET</td>
<td>Gaussian</td>
<td>$0.5P_e^{p}e^{-(x-x)^2/2P_2}$ erf $(x - X + \sqrt{2}aP_2) + 0.5P_e^{p}e^{-(x-x)^2/2P_2} erf (x - X - \sqrt{2}aP_2)$</td>
<td></td>
</tr>
<tr>
<td>S10</td>
<td>Campbell and Jorch (1979)</td>
<td></td>
<td>Gaussian</td>
<td>$P_e^{p}e^{-(x-x)^2/2P_1^2}$ for $x &lt; P_2 - 2P_1^2/P_1$</td>
<td></td>
</tr>
<tr>
<td>S11</td>
<td>Helmer and Lee (1980)</td>
<td></td>
<td>Gaussian</td>
<td>$P_e^{p}e^{-(x-x)^2/2P_1^2}$ for $x &lt; P_2 - 2P_1^2/P_1$</td>
<td></td>
</tr>
</tbody>
</table>

Symbols:
- $x$ = channel number (or independent variable),
- $X$ = center of the peak (in channels),
- $Y$ = Gaussian amplitude (in counts),
- $w$ = FWHM,
- $\sigma$ = Gaussian width parameter, $w = (8 \ln 2)^{1/2}a$,
- $J$ = distance (in channels) from peak center to junction point where Gaussian function changes to exponential function,
- $P_1$, $P_2$, ... = parameters to be determined from fit to experimental data, and erfc = complementary error function.
3.1.3 Shape of the peaks

Ideally, a full-energy peak can be represented quite accurately by a Gaussian function

\[
f(x) = Y \cdot e^{-(x-X)^2/2\sigma^2}
\]

(3.1a)

where \(Y\) is the amplitude, \(X\) the centroid, and \(\sigma\) the half-width at \(Y/\sqrt{e}\). The FWHM, \(w\), is related to \(\sigma\) by \(w = 2.35\sigma\). Alternatively, this expression can be written as

\[
f(x) = \frac{N}{\sqrt{\pi} \sigma / (4 \ln 2)} \cdot e^{-(x-X)^2/2\sigma^2}.
\]

(3.1b)

where \(N\) is the peak area. In practice the peak will have some tailing on the low-energy side and possibly on the high-energy side (primarily at high count rates).

The detail to which one is interested in the shape of a full-energy peak depends on the goals of the peak evaluation. For single peaks, any analysis, precise or routine, can be carried out with limited consideration of the peak shape. Simple peak representations will also be satisfactory in cases where the peak-to-background ratios are small (e.g., samples with very little activity) so that the tailing is lost in the background statistics.

However, there are many cases where these simple representations are not sufficient. It is clear from the shape of the peak in fig. 3.9 that if a weaker component occurs in the tailing region, it will be difficult to determine the energy and area of the lower energy peak without a knowledge of analytical functions that adequately represent the shape of the peak and the spectral background. Some of the many functions suggested to represent the deviation of the peak shape from a Gaussian are given in table 3.2. (For additional shape functions see Helmer and Lee 1980 and the references therein.) Most of these functions consist of a main Gaussian component plus an additive term or terms to account for the low-energy tailing. However, a few of the functions modify the main Gaussian to account for the tailing, such as function S2 in the table. Functions S7 and S8 modify the main Gaussian component and also have an additive tailing term. Although it is given here with one tailing term, the function S3 is often used with two tailing terms of the same form, but different amplitudes and slopes. The functions in table 3.2 have various numbers of parameters from the 3 (position, height and width) of the Gaussian to 8 or 9 for the expressions with two additive exponential tailing terms. We have not included any high-energy tailing term in these expressions, but such a term would be similar in form to the low-energy tailing term, except reflected about the peak centroid. While the parameters of a function used to represent the low-energy tailing should depend only on the \(\gamma\)-ray energy, those for the high-energy tailing will depend on the count rate and possibly the \(\gamma\)-ray energy.

Comparisons of how well most of these functions fit experimental data have been reported by McNeiles and Campbell (1975) for peaks at 14 and 514 keV and by Helmer and Lee (1980) for peaks at 1332 keV. More limited comparisons have been made by Lederer (1969), Joch and Campbell (1977) and Campbell and Joch (1979). The data in table 3.3 show how the \(\chi^2_R\) value varies for fits to 514- and 1332-keV peaks for several of these functions. Only the most complex functions fit these data with close to the precision of the statistics on the data points; that is, only the last few functions have \(\chi^2_R\) close to 1.0. All of the \(\chi^2_R\) values would be closer to unity if there were fewer counts in the peaks; for peaks with \(= 5 \cdot 10^4\) counts, one would expect little difference in the \(\chi^2_R\) for the expressions with

<table>
<thead>
<tr>
<th>Additive tail</th>
<th>Peak-shape parameters</th>
<th>Peak-shape function</th>
<th>Background step</th>
<th>(\chi^2_R)</th>
</tr>
</thead>
<tbody>
<tr>
<td>components</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>3</td>
<td>S1</td>
<td>yes</td>
<td>49.4</td>
</tr>
<tr>
<td>0</td>
<td>4</td>
<td>S7 c</td>
<td>no</td>
<td>17.6</td>
</tr>
<tr>
<td>0</td>
<td>4</td>
<td>S2</td>
<td>no</td>
<td>14.7</td>
</tr>
<tr>
<td>1</td>
<td>5</td>
<td>S4</td>
<td>yes</td>
<td>9.4</td>
</tr>
<tr>
<td>1</td>
<td>6</td>
<td>S4</td>
<td>yes</td>
<td>2.6</td>
</tr>
<tr>
<td>1</td>
<td>6</td>
<td>S8</td>
<td>yes</td>
<td>8.0</td>
</tr>
<tr>
<td>1</td>
<td>7</td>
<td>S3</td>
<td>yes</td>
<td>4.4</td>
</tr>
<tr>
<td>1</td>
<td>7</td>
<td>S10</td>
<td>yes</td>
<td>7.3</td>
</tr>
<tr>
<td>2</td>
<td>7</td>
<td>S4 + S4</td>
<td>yes</td>
<td>3.15</td>
</tr>
<tr>
<td>2</td>
<td>7</td>
<td>S5</td>
<td>yes</td>
<td>2.52</td>
</tr>
<tr>
<td>2</td>
<td>8</td>
<td>S9</td>
<td>yes</td>
<td>2.4</td>
</tr>
<tr>
<td>2</td>
<td>8</td>
<td>S11</td>
<td>yes</td>
<td>1.2</td>
</tr>
<tr>
<td>2</td>
<td>8</td>
<td>S9 + S4</td>
<td>yes</td>
<td>1.77</td>
</tr>
<tr>
<td>2</td>
<td>8</td>
<td>S11</td>
<td>yes</td>
<td>1.75</td>
</tr>
</tbody>
</table>

a See table 3.2 for definitions of these peak-shape functions.

b In Helmer and Lee (1980) values are given for fits to peaks from three detectors. The values here are from the detector with the intermediate size \(\chi^2_R\) values.

c Function S7 used without any additive tailing term.

d McNeiles and Campbell (1975) report this value for the function proposed by Dojo (1974), but the function is equivalent to S2 with a step-function background.
6 or more parameters. In interpreting these results, one should realize that the \( \chi^2 \) will depend critically on the range of channels used in a fit. This is especially true for the functions without additive tails (e.g., S1 and S2) where the \( \chi^2 \) values are very large. If one starts with a fitting range of a few channels near the peak, \( \chi^2 \) will increase as more channels in the tailing region are included, and then it will decrease as channels are included from the background. The fits considered here all involve a large channel range.

Fig. 3.11. Components of fit to a 1332-keV peak with the shape function S11, that is, two low-energy tailing terms and the erfc-type step background. The weighted residuals are shown in the lower plot (from Helmer and Lee 1980).

Fig. 3.12. Components of peak-shape function S11 (with high-energy tail added) fitted to a 2614-keV peak. The main Gaussian term is omitted for clarity (from McCullagh and Helmer 1982). — Short-term low-energy tail; ▲ Long-term low-energy tail; ‾‾‾‾‾‾ Step function background; ■ High-energy tail; ○ data

The contributions of the various terms of the shape S11 are shown in fig. 3.11 for a 1332-keV peak and in fig. 3.12 for a 2614-keV peak. Figure 3.13 shows how well the data for a 2614-keV peak are fitted by functions with an increasing number of parameters. Clearly, this peak is best fitted when two low-energy tailing terms and the high-energy tailing term are included.
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necessary to have available some spectra that contain strong, well-resolved peaks at several energies which span the energy range of interest. For these peaks one determines the parameters of the peak-shape function being used, and then from these results one determines analytical expressions that give these parameters as a function of the $\gamma$-ray energy. In the analysis of subsequent spectra these parameters would be fixed at their estimated values. Therefore, in the analysis of other spectra the only variable parameters would be those of the Gaussian component and the background. If a high-energy tail is included, the parameters would be functions of the count rate rather than, or in addition to, the energy.

The determination of the tailing parameters will usually need to be done with a separate nonlinear least-squares routine that is designed for this purpose. Especially for the shapes with two tailing terms, it is not easy to make good estimates of the initial values of the parameters and, as a result, the nonlinear fitting process may not always converge. Also, some experimenting may be necessary to obtain parameter values that vary smoothly with the peak energy. It should be much easier to determine consistent values for the functions with fewer parameters, for example, with only one tailing term.

The use of the more complex peak-shape functions may imply the need for a large computer to analyze the spectral data. However, Prussin (1982) pointed out that with most of these functions analyses are clearly possible on the current small computers as well.

It should be noted that even if the continuous pulse-height distribution at the input to the ADC closely approximates a Gaussian function, the distribution produced by the analyzer is distorted because of the creation of a discontinuous histogram. The multichannel analyzer combines in one channel all pulses with amplitudes in a range equal to the channel width, and the mean amplitude does not correspond to the center of the channel where the peak fitting places it, but nearer to the peak centroid. To minimize this distortion, it is important that the FWHM is large enough, say, at least 4 or 5 channels. The $x^2$ of a fit to a very narrow peak would be expected to be much larger than unity.

In some cases it is possible to change the form of $f(x)$ in eq. (3.1) and as a result replace the nonlinear by the linear least-squares method. This is possible if a simple Gaussian function, without any tailing terms, suffices for a fit, and the spectral background can be subtracted before the peak is fitted. Then the total fitting function is a Gaussian, whose logarithm is

$$
\ln[f(x)] = \ln(Y) - \frac{(x - X)^2}{2\sigma^2}
$$

$$
= \ln(Y) - X^2/2\sigma^2 + \left(\frac{X}{\sigma^2}\right) \cdot x - \left(\frac{1}{2\sigma^2}\right) \cdot x^2. \quad (3.2a)
$$
This is a linear fitting problem since with \( a_1 = \ln(Y) - X^2/2 \cdot \sigma^2 \), \( a_2 = X/\sigma^2 \), and \( a_3 = 1/2 \cdot \sigma^2 \), one has

\[
\ln[ f(x) ] = g(x) = a_1 + a_2 \cdot x + a_3 \cdot x^2
\]

with the \( a_i \) to be determined in the fit.

In our discussion we have, thus far, referred directly only to full-energy peaks, but the same ideas apply to single- and double-escape peaks. However, since the single-escape peaks contain the same broadening component as the 511-keV annihilation radiation, one must take into account the fact that they are wider than the full-energy peaks. This distinction is especially important if the widths of the peaks are fixed during the peak fitting process to the values obtained from a width function; that is, a different function would be needed for the single-escape peaks.

### 3.2 Peak location

Several methods have been developed for the automatic location of the peaks in a spectrum. Although the visual location of peaks may still be the best method, automatic routines are of particular value when there is a large number of peaks to be located in a spectrum, or when many spectra are to be analyzed. The sensitivity of any search routine can be varied to have it find more or fewer “peaks” at the user’s discretion. But, as the routine is pushed to obtain more of the small, but real peaks, it will naturally find more “peaks” that are statistical fluctuations, or structure in the spectral background, rather than real peaks. Therefore, any spectral analysis plan must define the optimum sensitivity of the automatic peak-location routine. For interactive computer programs, the number of peaks found can be controlled by having the user edit the results of the peak-location routine to add or delete entries. As will be discussed in section 5.1.4, it is also possible to use a peak-fitting routine that can increase the number of peaks in a region of the spectrum. This can be very effective in compensating for peaks missed in the search process.

Mariscotti (1967) developed a peak-location method that involves the second derivative of the spectrum. As illustrated in fig. 3.14, in the second derivative a large negative peak and two smaller positive peaks are the signature for the presence of a peak, and the peak location corresponds to the minimum of the negative peak. At the same time, a smooth background gives a constant first derivative and then a zero second derivative. By applying selection criteria based on the statistics of the data, one can suppress the statistical fluctuations and thus identify the peaks. The peak

with two or more components will give a more complex array of positive and negative peaks in the second derivative for which the number and spacing depends on the number of \( \gamma \)-ray components and their spacing. In principle, a Compton edge can be distinguished since it will give a second derivative with one positive peak rather than two. By use of coding to distinguish between these various patterns, the peak-location routine can discriminate out the Compton edges and determine the approximate number of peak components. For multiplets the success of the routine will depend greatly on the separation of the components compared to the FWHM of the peaks. This method has been widely applied, for example, it is used in the computer codes SAMPO (Routti and Prussin 1969) and GAMANAL (Gunnink and Niday 1972).

In order to take meaningful derivatives of data with statistical fluctuations, it is necessary to smooth the data before the derivatives are taken, or to use some generalized expression for the derivative that has the effect of smoothing it. Expressions for the smoothed second derivative, and the optimum choice of the values of the parameters in it, have been discussed by Mariscotti (1967).

A correlation method for peak location was developed by Black (1969) and Connelly and Black (1970). It is an approach that is the opposite of the derivative methods in that it attempts to emphasize the Gaussian structures.
Fourier transform methods for smoothing the spectrum by removing the high-frequency components in the transform and thereby aiding in finding peaks were discussed by Harper et al. (1968). Other methods of finding peaks have been described by Slavíc and Bingulac (1970) and Bullock and Large (1971). Recently, Lauterjung et al. (1985) have described a search method that also provides a decomposition of multiple peaks into their components.

For any peak-location routine, the user should test its sensitivity as a function of any control parameter and of the number of counts in the spectrum. It should be expected that the sensitivity will vary with the number of counts in a manner that is different from that of visual inspection. For example, the routine may find "peaks" the user can not see on the usual log plot for large counts and still miss peaks the user can easily identify for small counts. Such tests are especially important for a commercial routine where the details of the method may be unknown.

The above peak-location processes may give the location only to an integer channel. If so, before initiating the peak analysis, it may be useful to improve this value. This can be done simply by fitting a quadratic function \( a_3 + a_2 \cdot x + a_1 \cdot x^2 \) to the log of the count or the net counts (i.e., \( y \) minus some estimated spectral background) for a few points around the peak. The point at which the derivative \( dy/dx \) is zero, \( X = -a_2/2 \cdot a_3 \), gives the peak location. This method should give the peak location to 0.1 channels, if the statistical quality of the data allow that accuracy. This improvement should help the peak-fit process.

### 3.3 Peak evaluation

For the analysis of most \( \gamma \) - and X-ray spectra the goal is to determine the emission rates of the photons. For this purpose the quantities needed from a spectrum are the number of counts in the full-energy peaks. The methods that can be used range from the simplicity of adding up the counts in a few channels to the complexity of fitting the counts in a group of channels by means of the nonlinear least-squares method with one of the shape functions discussed in section 3.1.3.

Any method can be used to obtain precise peak areas if the spectrum involves single or completely resolved peaks. However, as discussed in section 3.3.2, this does not mean that the peak area is a well-defined quantity and that each method will provide the same value. In fact, the opposite is the case. The "area" is an ill-defined quantity, and different methods will determine different values, therefore, the area of a peak is defined, in part, by the method used to compute it. The quality of an
analysis depends on how reproducible the method is, rather than on the actual area obtained. The reason that the user has some flexibility in how he defines the area, and still get correct answers, is that the detector efficiency function (see section 4.2) is determined with the same peak-fitting methods. Therefore, any differences among the methods used in computing the area of a particular peak will show up in both the analysis of an unknown spectrum and the analysis of the efficiency-calibration spectra.

As a test of the quality of analysis programs, the IAEA coordinated an international comparison of the results from peak-location and peak-area analysis methods. Spectra, which were constructed so that they had peaks with known areas and positions, were distributed to spectroscopists who analyzed them with their standard methods. This set of test spectra, which is still available, includes both large and small peaks, so several phases of a program can be tested. Parr et al. (1979) and Zagyvai et al. (1985) report results of this study. Nielsen (1982) has used these spectra more recently for a test of the quality of an analysis program.

### 3.3.1 Simple peak-area-evaluation methods

There are many specific methods that have been used to “simply” add up the counts in a peak. Several of these have been discussed in the reviews of Kokta (1973) and Hertogen et al. (1974). Specific summation methods are also discussed by Quittner (1969), Laitano et al. (1979), and Yule and Rook (1977). In these methods a significant question is how, procedurally and statistically, to define both the spectral background that is to be subtracted and the uncertainty in the computed area. See Hertogen et al. (1974) for detailed conclusions concerning these methods.

For large peaks, the total uncertainty of the area depends mostly on the reproducibility of the analysis method, that is, on the ability to control the channel range for the summation. Hirshfeld et al. (1976), Schima et al. (1979) and Debettin (1980) have used summation methods for precise γ-ray emission rate measurements. Their procedures are as follows. First, the approximate peak position is determined and a range of channels on either side is chosen to define the background under the peak. The background is taken to be a linear function, but, in principle, could be more complex. The peak region is fitted with a Gaussian function primarily to determine the peak width \( w \) (i.e., FWHM), and secondarily to determine the peak position \( x \) and the Gaussian area \( N_p \). Then the gross summation area \( N_s \) is determined by adding up the counts in a definite range centered at \( x \).

Reasonable choices for this summation range are from \( 2 \cdot w \) to \( 3 \cdot w \). For a range of \( 2.55 \cdot w \), \( 99.7\% \) of the area of a pure Gaussian function would be included. Since the ends of the summation range will not be integer

channels, it is necessary to account for the fraction of channels at the ends by including in the summation the appropriate fraction of the count from the end channels. The background, \( N_b \), can be taken from summation intervals to the left, \( N_{b,l} \), and right, \( N_{b,r} \), of the peak, with widths equal to one-half that of the peak range. This method is illustrated, with some simplification, in fig. 3.16. The net count, \( N \), is obtained from \( N = N_s - N_b \).

The uncertainty in \( N \) can reasonably be taken as \( \sqrt{N_s + N_b} \).

If the value of \( w \) comes from the peak being analyzed, any distortion of the peak (e.g., due to electronic drift) will be taken into account. Also, since the percentage of the pure Gaussian area included in the summation is very close to 100%, any such distortion should influence the area by only a very small percentage. For a small peak, as shown in fig. 3.16, the summation range should be computed from the width function determined from the stronger peaks rather than the value from fitting this peak.

Some routines may carry out a summation calculation of the peak area in a still more simplistic manner. For example, the user may place two markers on the spectrum – one below the peak and one above it. The routine then adds the counts in the channels between the markers and subtracts a background which is equivalent to that under a straight line between the counts in the marked channels. One should expect that the areas from such a method will be less reproducible than those from the method suggested above because the choice of the marker channels is more subjective and the background is less accurate due to the use of only two channels.
3.3.2 Peak areas from analytical fitting

The peak area can also be obtained with a computer program that fits an analytical function, such as those noted in section 3.1.3, to each peak. The parameters that define the tailing and the height of the step should be determined from prior measurements. A nonlinear least-squares fitting routine can then be used to determine the Gaussian parameters, that is, the peak position, amplitude or area, and width as well as the parameters of the background function, in the simplest case the intercept and slope of a linear function. In some cases the background and/or the peak width are/is fixed at a predetermined value and not varied in the fitting process.

The peak area can be taken as the integral of the appropriate part of the analytical function. For a simple Gaussian as described in eq. (3.1a), the area is

$$ N = Y \cdot w \cdot \sqrt{\frac{\pi}{4 \cdot \ln 2}}. $$

(3.4)

If a Gaussian is described as in eq. (3.1b), the area results directly as the parameter $N$ from the fitting process. If the peak-shape function includes one or more tailing terms, the experimenter must decide how much, if any, of the area under these tailing functions is to be included in the peak area. For some functions the choice is clear, such as for the exponential term used in the SAMPO program (S2 in table 3.2). In this case part of the Gaussian is replaced by an exponential, so the only useful choice is to include the area under the exponential. If two low-energy tailing terms are used, it would be quite reasonable to include the area under the short-term tail in the peak area, and to consider the long-term tail as part of the spectral background. The choice may be more ambiguous if the relationship of a tailing term to the Gaussian component varies considerably from one detector to another, so that the tailing component may be mostly in the peak or mostly in the spectral background depending on the quality of the detector. This variability may occur with functions that have one tailing term, and it will require careful consideration by the user of the definition of the area.

It is of interest to note the magnitude of the differences that can occur in the calculated area for a particular peak. For this purpose we have fitted various functions to a 1332-keV peak. The results in table 3.4 show a 2.6% variation in the peak area. Although this variation is large compared to the reproducibility that might be expected in precise spectrometry ($\approx 0.1\%$), it is not important as long as one uses one peak-shape function and analyzes spectra in a reproducible manner.

The area obtained with a function that does not properly fit the tailing, as the simple Gaussian, will depend markedly on the range of channels used in the fit. The fact that in the above example the simple Gaussian, S1, gives an area comparable to the other functions is due in part to the use of a broad fitting range such that the data points in the tailing region force the Gaussian amplitude up and thereby increase its area to a value that is comparable with the total area of the other functions. Among the different functions the area of the main Gaussian component varies by very large amounts, it is particularly low for the shape S9 where the short-term tailing component competes with the Gaussian for the counts in the main peak. Although this large variation is not of practical concern as long as one includes the short-term tailing in the area, one should be aware of it.

As a measure of the quality of the fits for single peaks, the results of an automatic analysis (with the GAUSS VII program) of the strong peaks in a $^{188}$Ta spectrum are compared in table 3.5 with a careful, manual, interactive analysis. The fitting functions were simple Gaussians, so the fits are somewhat more sensitive to the choice of the channel range than they might be if this function included a low-energy tailing term. The automatic fits were done with both variable and fixed widths, while the interactive fits were carried out only with a variable width. In the interactive analysis, the counts representing the background on either side of the peak were chosen by the analyst and were fixed during the fitting process. This background was a step-like function. Also, in the interactive analyses, the fit only included the data from one FWHM below to one FWHM above the centroid. Although this smaller fitting range of the interactive analyses might result in a systematically different area, the ratios of the GAUSS VII areas and the interactive areas should vary only slowly with the peak
Spectrum analysis and energy measurements

Table 3.5

<table>
<thead>
<tr>
<th>Energy (keV)</th>
<th>N₁</th>
<th>N₁/N₂ν</th>
<th>N₁/N₂η</th>
</tr>
</thead>
<tbody>
<tr>
<td>32</td>
<td>196744</td>
<td>1.007</td>
<td>1.018</td>
</tr>
<tr>
<td>43</td>
<td>57522</td>
<td>1.039</td>
<td>1.001</td>
</tr>
<tr>
<td>85</td>
<td>623952</td>
<td>0.950</td>
<td>0.992</td>
</tr>
<tr>
<td>100</td>
<td>3101499</td>
<td>0.997</td>
<td>1.014</td>
</tr>
<tr>
<td>114</td>
<td>371872</td>
<td>0.996</td>
<td>0.996</td>
</tr>
<tr>
<td>116</td>
<td>87976</td>
<td>1.002</td>
<td>1.003</td>
</tr>
<tr>
<td>152</td>
<td>997545</td>
<td>0.998</td>
<td>0.998</td>
</tr>
<tr>
<td>156</td>
<td>360181</td>
<td>0.995</td>
<td>0.995</td>
</tr>
<tr>
<td>179</td>
<td>338903</td>
<td>1.001</td>
<td>1.001</td>
</tr>
<tr>
<td>198</td>
<td>134786</td>
<td>1.003</td>
<td>1.005</td>
</tr>
<tr>
<td>222</td>
<td>573111</td>
<td>1.000</td>
<td>1.001</td>
</tr>
<tr>
<td>229</td>
<td>260822</td>
<td>1.001</td>
<td>0.999</td>
</tr>
<tr>
<td>264</td>
<td>200621</td>
<td>1.001</td>
<td>0.999</td>
</tr>
<tr>
<td>1121</td>
<td>208737</td>
<td>1.009</td>
<td>1.005</td>
</tr>
<tr>
<td>1189</td>
<td>92215</td>
<td>1.011</td>
<td>1.006</td>
</tr>
<tr>
<td>1221</td>
<td>146434</td>
<td>1.046</td>
<td>1.016</td>
</tr>
<tr>
<td>1231</td>
<td>61522</td>
<td>1.014</td>
<td>1.010</td>
</tr>
<tr>
<td>Average</td>
<td>1.004</td>
<td>1.004</td>
<td></td>
</tr>
</tbody>
</table>

Symbols:
N₁ = area from interactive fit with FWHM variable,
N₂ν = area from GAUSS VII fit with FWHM variable,
N₂η = area from GAUSS VII fit with FWHM fixed.
Data are from McCullagh and Helmer (1982).

energy.

The agreement in table 3.5 is quite good, with the average ratio of 1.004 for either the variable- or fixed-width fits. The largest deviations, ±5%, are for the variable-width automatic fits. This is expected since the Gaussian width and the background can at times change cooperatively to increase or decrease the computed area. For the 85-keV line, the deviations of 5% and 0.8% are certainly due to a poor representation of the background which is not linear as the fitting function assumes. In contrast to the deviation of −5.0 to +4.6% for the variable-width fits, the extreme deviations from the fixed-width fits are +1.8 and −0.8%. The data in table 3.5 suggest that a precision of 1 to 2% can be obtained even with automatic analyses in regions of a spectrum that are quite simple as is the case for the 182Ta spectrum.

The definition of the peak area may affect the pile-up corrections discussed in section 4.6. Random summing of amplifier pulses produces counts in the region above a full-energy peak. If the calculated area includes the area under a high-energy tailing term, or if a summation method is used, this area will include some of the random-summing events. Therefore, the magnitude and energy dependence of this correction will depend in part on how many of the summed events are included in the peak area.

In subsection 3.1.2 we have made the point that we consider the step as a part of the spectral background; that is, the area under the step is not part of the peak area. However, in the analysis process, the amplitude of the step may be given as a specified fraction of the peak amplitude so that the step is part of the peak-shape function. This is desirable in that it means that the amplitude of the step will not be a variable parameter. At low energies one must be very careful with such a process because a major contribution to the step may be from scattering of the photons from the material surrounding the source of detector (see sections 2.3.3 and 4.2.2), so the amplitude of the step may vary with source–detector geometry and with the amount of material in the source.

In an analysis of a peak or a group of peaks, it is reasonable to assume that the computer program will calculate the variances of the resulting parameters. If a peak is represented by a Gaussian function as given in eq. (3.1b), the uncertainty in the area is given directly since it is one of the parameters. If expression (3.1a) is used, the uncertainty in N can be computed from the variances in Y and w and their covariance. If the background is not varied in the fit, other contributions need to be added to account for the uncertainty in the background. If tailing is included in the peak-shape function, additional contributions are needed to account for the uncertainty in the area under the tail.

As discussed in section 1.6.4, the strict validity of the calculated variance of N is limited to situations where the actual peak shape is well represented by the chosen fitting function. Since the var terms include a factor of χ², they will increase whenever this function does not fit the data well. As shown in table 3.6, the value of χ² can increase dramatically as the number of counts in the peak increases. This means that the relative uncertainty in N does not necessarily decrease as the statistical quality of the data improves. Although it is true that this increase in χ² does represent a failure of the function to fit the peak, it is not necessarily pertinent in certain γ-ray intensity measurements. As noted above, it is the reproducibility of the peak-area calculation that is usually the important factor. Therefore, the experimenter should carefully consider if this χ² value should be included in the uncertainty. For example, it might be deleted in computing an activity ratio of two 60Co sources, since the same discrepancy between the data and the fit function occurs for each source.
Spectrum analysis and energy measurements

Comparison of $\chi^2$ values for fits to peaks with increasing areas, $N$, and the effect on the computed uncertainty in the area. (Data from Lederer 1969 and Helmer et al. 1971)

<table>
<thead>
<tr>
<th>$N$ (counts)</th>
<th>Uncertainty as $\sqrt{N}/N$ (%)</th>
<th>Fit with S1</th>
<th>Fit with S2</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2.5 \cdot 10^2$</td>
<td>6.5</td>
<td>0.85</td>
<td>0.77</td>
</tr>
<tr>
<td>$5.1 \cdot 10^2$</td>
<td>4.5</td>
<td>1.94</td>
<td>1.76</td>
</tr>
<tr>
<td>$2.6 \cdot 10^3$</td>
<td>2.0</td>
<td>0.78</td>
<td>0.67</td>
</tr>
<tr>
<td>$1.3 \cdot 10^4$</td>
<td>0.93</td>
<td>1.40</td>
<td>0.77</td>
</tr>
<tr>
<td>$5.1 \cdot 10^4$</td>
<td>0.46</td>
<td>3.4</td>
<td>1.34</td>
</tr>
<tr>
<td>$2.5 \cdot 10^5$</td>
<td>0.21</td>
<td>8.9</td>
<td>2.30</td>
</tr>
<tr>
<td>$1.3 \cdot 10^6$</td>
<td>0.09</td>
<td>47.0</td>
<td>9.1</td>
</tr>
</tbody>
</table>

* If $\chi^2$ is less than 1.0, then the uncertainty is $\sqrt{N}/N$.

Although in precision measurements all three parameters of the main Gaussian are usually varied, there are many other cases in which the peak width is fixed at its initial value. In this case the $\chi^2$ value may be increased, from the statistically expected value of 1.0, both by the peak shape not fitting the data as discussed above, and by the width not being the optimum value. From the arguments in the previous paragraph, it may be acceptable to neglect that from the former contribution to $\chi^2$, but it is not suitable to neglect that from the width being incorrect. In this situation, as in all cases, the experimenter must be certain that the reported uncertainty is a realistic value for his purposes.

### 3.3.3 Analysis of multiple peaks

In this section we indicate some special features of the analysis of multiplets. It is evident that the simple summation method, described in subsection 3.3.1 can not provide the areas of the individual peaks of an unresolved multiple peak. Clearly, with this method we can determine the total area of a multiple peak, but this is only useful if the spectrometrist has some independent method to partition the total area between the components. (Some of such methods are discussed in sections 5.2.3 and 5.1.6.)

The fitting methods, on the other hand, can be easily extended to the case of a multiple peak. For a doublet, for example, the fitting function is the sum of two functions that are identical in shape, but with different values of the parameters. For the simplest case of Gaussian functions, we get

$$f(x) = Y_1 \cdot e^{-(x-x_1)^2/2\sigma^2} + Y_2 \cdot e^{-(x-x_2)^2/2\sigma^2}.$$  \hspace{1cm} (3.5)

Instead of three, now five parameters ($Y_1$, $Y_2$, $x_1$, $x_2$, and $\sigma$) have to be fitted. (Note that $\sigma$ has been assumed to be the same for both peaks.)

Normally, these analyses will be carried out by nonlinear least-squares fitting since both $w$ or $\sigma$ and $X$ occur nonlinearly. However, Mukoyama (1981) has described a linearization method for analyzing doublet peaks, so that a linear, rather than a nonlinear least-squares fit can be used.

In order to analyze multiple peaks accurately, usually one must represent the peaks and the background with functions that are better approximations to the observed shapes than the simple Gaussian functions. This is clear from the example of a doublet peak in fig. 3.17. A fit of two components to this pulse-height distribution will only yield a reliable peak area and position for the small peak, if the tail in the function has been chosen properly. Our earlier comment that the reproducibility of the analysis method is more important than the exact reproduction of the peak shape is valid for single peaks, but not for multiplets. There will be an error in the area of the smaller peak from not using the proper shape for the larger peak. This is not reflected in the $\chi^2$ value, and generally it will not show up in the computed uncertainty in this area; that is, it is an error and not an uncertainty.

The range of channels in the analysis of a singlet is important in determining whether one obtains consistent areas from the fits to singlets.
and multiplets. If this range does not include the tailing region, the fit of a multiplet where a particular peak is a part of it, will almost certainly result in a different area from that for this peak when it is fit as a singlet.

Some commercial systems have used one method for single peaks and a different method for multiplets, for example, a summation method for single peaks (because it is fast) and a fit with Gaussian functions for multiplets. Furthermore, when a Gaussian function is used, the three parameters (amplitude, position and width) are not necessarily allowed to vary. Instead, the peak widths may be taken from a calibration function and the peak positions from the results of the peak-location routine. This makes the calculation a linear least-square problem since only the peak amplitudes or areas are varied. For members of a multiplet, there can be a significant error in the peak locations from the search routine, and this may result in significant errors in the peak areas as well. This limitation, and the possible inconsistency in the ways different peaks are analyzed, introduces errors in the results that will not be reflected in statistical computations of the uncertainties. Therefore, it is important that each user understands the methods on which his analysis program is based.

For a given peak analysis code, its ability to correctly compute the area of the individual components of a multiplet can be tested by applying the code to an artificially constructed multiplet where the ratios of the peak areas are known. Such a multiplet can be synthesized by accumulating the counts in a single peak over a definite time period, changing the amplification in the electronics slightly, continuing the accumulation for a further known time period, changing the amplification again, etc. By this procedure real multiplets can be produced.

3.3.4 Shape and analysis of X-ray peaks

Most of the principles discussed above also apply in the analysis of full-energy peaks from X rays, however, there are some additional aspects that deserve consideration. First, these peaks are usually multiplets. But, often one does not need the separate areas for the different X-ray components since their relative intensities are already known. Therefore, a summation method that takes into account the spectral background may be quite satisfactory, as long as there are no interfering lines. If a fitting program is used to obtain the peak areas, the program must deal with this multiplicity of components. This is straightforward for the $K_\alpha$ peaks since they can have only 2 components, but it is more complex for the several components of the $K_\beta$ and the L X rays.

The second new consideration is that the widths of the emitted X-ray lines are orders of magnitude larger than those of the $\gamma$ rays, and are no longer negligible in comparison with the FWHM, $\sigma$, introduced by the detector system. As discussed in section 3.3.1, the natural line shape can be represented by a Lorentzian function

$$L(E) = \frac{1}{2\pi} \frac{1}{(E - E_0)^2 + (\Gamma/2)^2}. \quad (3.6)$$

where $E$ is the energy, $E_0$ is the mean energy, and $\Gamma$ is the line width. This function has very far-reaching tails that lead to a deviation of the observed peaks from a Gaussian in the tail regions. This is illustrated in fig. 3.18 for 88-keV $\gamma$ rays and lead K X rays at 72.8 and 75.0 keV. The convolution of the line profile $L(E)$ with the spectrometer response function, for which we assume a Gaussian function $G(E)$, results in a Voigt function

$$V(E) = \int_{-\infty}^{\infty} L(E') \cdot G(E - E') \, dE'. \quad (3.7)$$

In fig. 3.19 the right halves of the Lorentzian, Gaussian, and Voigt functions are shown for $E_0 = 75$ keV, $\Gamma = 62$ eV, and $\sigma = 450$ eV, which are typical values for the measurement of lead X rays with a planar Ge detector. With these parameters the Gaussian dominates the shape of the Voigt function over the top portion, while the Lorentzian dominates for amplitudes of less than 1% of the peak amplitude.

The problems related to fitting Voigt functions to observed peak data have been discussed by, for example, Wilkinson (1971), Gunnink (1977) and Schulte et al. (1980). These authors developed algorithms to generate the Lorentzian-broadened distributions by either using analytical approximations to the Voigt function or by numerical methods.

If the X-ray multiplets need not be resolved, the peak analysis can be confined to the simple summing of the counts in a definite interval around the multiplet, as described in subsection 3.3.1. However, in this case the channel range will not include the same fraction of the counts as for $\gamma$ rays. The summation interval from $E_0 - 3 \cdot \sigma$ to $E_0 + 3 \cdot \sigma$ ($\sigma = 2.35 \cdot \sigma$) covers 99.7% of the total area of a pure Gaussian, but only 95.7% of a Voigt function with the parameters illustrated in fig. 3.19 (Debertin and Pessaro 1981). For other $\Gamma/\sigma$ ratios and summation intervals, Wilkinson (1971) has calculated the corresponding percentages. If one summation interval includes two X-ray peaks, this interval becomes asymmetric for each peak and the fraction in the summation interval increases. The effect of the natural line width can be neglected for measurements of limited precision if the atomic number $Z$ of the X-ray emitter is low or in spectra with small peak-to-background ratios. However, there are many measurements where
the X-ray emitters are of high Z, the spectra are of high quality, and where precise results are desired. Here this effect must be taken into account.

In addition to the Lorentzian tails, full-energy peaks from X-rays show, as for γ rays, low-energy tailing due to incomplete charge collection. This is discussed in general for low-energy photons in section 4.2.2. A further contribution to this tailing results from Compton scattering of source photons in the material surrounding the detector (see section 2.3.3). At X-ray energies below 15 keV, one also has contributions to the tailing from the radiative Auger effect (see sections 1.3.2 and 4.2.2).

Campbell et al. (1985) performed careful peak-shape measurements with single K- and L-X-ray lines that were selected by Bragg diffraction from a curved crystal. This method produces a monoenergetic beam so the observed spectrum is the pure response function, and the parameters for the tail function can be derived more accurately than possible with the usual X-ray multiplets. These authors and others (e.g., Watanabe et al. 1986) concluded that some of the functions in table 3.2 (e.g., S9) are well suited to describe full-energy peaks from X rays, provided that the natural line widths are negligible compared to the observed peak widths. Special computer programs written for the analysis of X-ray spectra are reported by
Van Espen et al. (1977), Marageter et al. (1984b), Arthur et al. (1984) and Petersen et al. (1986).

An alternative method of analyzing X-ray peaks, that makes use of the known relative peak positions and known relative intensities and does not require the shapes of single peaks, is discussed in section 5.2.3.

3.4 Energy calibration

The brief history of γ-ray spectrometry given in section 1.2 includes a discussion of earlier energy scales and the development of sets of energy-calibration lines. In this and the following section, the current methodology of γ-ray energy measurements is described. The topic is presented both in terms of precise and routine measurements. In routine measurements the same general methods should be used, but less care to details is needed. However, each spectrometrist should be aware of all the parameters that influence his measurements so that the associated uncertainties are understood.

3.4.1 Energy scale

In this section we give details, both historical and technical, of the current recommended energy scale that are important for those involved in precise γ-ray energy measurements. For routine measurements these details are not important since the spectrometrist can use any set of recently evaluated photon energies (e.g., Browne and Firestone 1986, NCRP 1985, Helmer et al. 1979). Such readers may wish to proceed to section 3.4.2.

By 1978 the current system of energy-calibration standards had begun to develop as a result of the availability of a new set of very precise γ-ray wavelengths. Kessler et al. (1978) and Deslattes et al. (1980) made a series of measurements at the NBS that related the wavelengths of several γ rays to the wavelength of the optical radiation that defines the meter. These measurements involved the following steps:

- the determination, in terms of the meter, of the lattice spacing of some pure Si reference crystals,
- the determination of the lattice spacing of some thicker Si crystals relative to the reference crystals, and
- the measurement of some γ-ray wavelengths by Bragg diffraction with the second set of Si crystals.

The results of these measurements, given in table 3.7, have uncertainties in the wavelengths of 0.26 to 1.5 ppm. In contrast to the earlier problems with wavelength scales of x-units and Å*-units, these wavelengths are directly related to the meter.

It would be possible, and logically even desirable, to use these wavelengths directly as calibration values and report all subsequent measurements in units of length (cm or pm). Such a procedure would maintain this precision. However, spectrometrists have preferred to continue the historical practice of using the energy scale (keV). On this energy scale it has been necessary to include an additional uncertainty of 2.6 ppm, since this was the uncertainty associated with the cm–keV conversion factor from the 1973 evaluation of the fundamental constants (Cohen and Taylor 1973).

### Table 3.7

<table>
<thead>
<tr>
<th>Source</th>
<th>Wavelength (10⁻¹² m)</th>
<th>Energy (keV)</th>
<th>Uncertainty (ppm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>¹⁹⁷Au</td>
<td>3.010 778 6</td>
<td>411.804 44</td>
<td>0.31</td>
</tr>
<tr>
<td>¹⁹²Ir</td>
<td>1.834 406 1</td>
<td>675.887 43</td>
<td>1.01</td>
</tr>
<tr>
<td></td>
<td>6.024 680 0</td>
<td>205.795 49</td>
<td>0.26</td>
</tr>
<tr>
<td></td>
<td>4.189 279 8</td>
<td>295.958 27</td>
<td>0.39</td>
</tr>
<tr>
<td></td>
<td>4.019 530 5</td>
<td>308.456 92</td>
<td>0.42</td>
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<tr>
<td></td>
<td>3.917 266 0</td>
<td>316.507 91</td>
<td>0.43</td>
</tr>
<tr>
<td></td>
<td>2.648 851 6</td>
<td>468.071 52</td>
<td>0.51</td>
</tr>
<tr>
<td></td>
<td>2.558 622 2</td>
<td>484.577 99</td>
<td>0.83</td>
</tr>
<tr>
<td></td>
<td>2.106 497 8</td>
<td>558.584 51</td>
<td>1.17</td>
</tr>
<tr>
<td>¹⁶⁹Yb</td>
<td>2.051 326 9</td>
<td>604.414 64</td>
<td>0.34</td>
</tr>
<tr>
<td></td>
<td>2.024 361 7</td>
<td>612.465 64</td>
<td>0.33</td>
</tr>
</tbody>
</table>

| ¹⁷⁰Tm  | 19.642 536 1        | 63.120 77    | 1.34              | 2.93 |
|        | 13.244 139 6        | 93.615 14    | 1.26              | 2.89 |
|        | 11.293 982 7        | 109.779 87   | 0.48              | 2.64 |
|        | 10.490 313 2        | 118.190 18   | 1.53              | 3.02 |
|        | 9.499 057 7         | 130.523 68   | 0.28              | 2.61 |
|        | 6.996 354 0         | 177.214 02   | 0.32              | 2.62 |
|        | 6.263 211 2         | 197.957 88   | 0.32              | 2.62 |
| ¹⁷⁰Tm  | 4.748 961 3         | 261.078 57   | 0.44              | 2.64 |
|        | 4.028 926 4         | 307.737 57   | 0.28              | 2.61 |

* These values are weighted averages of the directly measured values and the values calculated from the energies (corrected for recoil) that sum to these values.
With the availability of the new values for the reference line energies in table 3.7, and especially the new value for the 411-keV line from $^{199}$Au, many previously reported energies for other $\gamma$ rays could be re-evaluated to this scale. Most of these values had been measured relative to the $^{199}$Au line with either a crystal spectrometer or a Ge detector. This process of evaluation and conversion to the new scale was done originally by Helmer et al. (1979). At the same time, Greenwood et al. (1979) reported many new $\gamma$-ray energy measurements that extended the set of available precise calibration lines from 1.3 MeV up to 3.5 MeV. Some of these calibration energies were given a more formal status by the publication of a set of recommended $\gamma$-ray energies by the Gamma-Ray Energy Task Group of the Commission on Atomic Masses and Fundamental Constants of the International Union of Pure and Applied Physics (IUPAP) (Helmer et al. 1979). The requirements that this Task Group established for the inclusion of a value were that the uncertainty was 10 ppm or less, that the measurement was well documented, that the $\gamma$-ray line was resolved in a Ge detector spectrum, and that (with only a few exceptions) it was from a long-lived radionuclide. This group was able to provide 125 energies from 67 keV to 3.45 MeV that met these criteria indicating that there were sufficient calibration lines available below 3.5 MeV. In section 6.3, table 6.6 gives many $\gamma$-ray energies that are useful in the calibration of semiconductor detectors.

In the first few years after the publication of this set of recommended $\gamma$-ray energies, there was little change in the situation. On the positive side, some additional precise measurements were made including additional wavelength measurements at NBS for the energies of the K-X-ray lines for several elements (Kessler et al. 1982) and $\gamma$ rays at higher energies than those in table 3.7 (Kessler et al. 1985) as well as other measurements for $\gamma$ rays at lower energies (25 to 74 keV) from the decay of $^{161}$Tb (Jeckelmann et al. 1985). On the negative side, a question arose concerning the accuracy of the Si-lattice-parameter measurement on which these values were based. A measurement by Becker et al. (1981) at PTB resulted in a different lattice spacing for pure Si crystals. Since this difference was 1.8 ppm, which is about 20 times as large as the uncertainty quoted for either measurement, it is very significant for the quoted wavelengths. However, this difference is smaller than the 2.6 ppm uncertainty in the wavelength-energy conversion factor, and, therefore, is less significant on the energy scale. Measurements that are currently being made will resolve this discrepancy. This fact and the availability of a new adjustment of the fundamental constants (Cohen and Taylor 1986 and 1987) will provide the basis for a revision of the precise $\gamma$-ray wavelengths and the energies on the keV scale that should become available in 1989. It is anticipated that the $\gamma$-ray energies will decrease by about 6 ppm.

While the wavelength and energy scales are now consistent, another scale for energies has taken on some interest. Since 1975 there have been available some very precise measurements of the difference in mass between various atoms or nuclei. These values can be used to establish, on the mass scale, the energies of some highly excited neutron-capture states as well as a few beta-decay $Q$ values. For example, Smith and Wapstra (1975) give a few measured mass differences with uncertainties of 1–2 ppm. When converted to the keV scale, the corresponding neutron-binding energies have uncertainties of 3–6 ppm. From measurements of the relative energies of the $\gamma$ rays that deexcite a neutron-capture level, the $\gamma$-ray energies can be established on the mass scale. There has been considerable interest in the question of whether this energy scale and that based on the wavelengths are consistent. Although this issue is not of concern, even for spectrometrists making precise measurements, it is of interest in the consideration of how well the definition of the keV scale is known. This matter has been discussed by Cohen and Wapstra (1983).

Due to their complex structure X-ray lines are usually not used for an energy calibration, but at times they may be useful. Over a long period of time, precise X-ray wavelength measurements, both absolute and relative, have been carried out including the recent measurements of Kessler et al. (1982). These results indicate (Kessler 1985) that the values calculated from the evaluated electron-binding energies of Sevier (1979) are accurate to about 1 eV for most elements. However, in any use of these values, the spectrometrist must consider the fact that the observed X-ray energies do depend on the chemical bonding (see section 1.2.3), that an X-ray line is broader than a $\gamma$-ray line of the same energy and that the X-ray lines have a different shape (see section 3.3.4 or 1.3.1).

### 3.4.2 Energy-calibration functions

For any spectrum in which there is a sufficient number of singlet peaks with known energies, the determination of the $\gamma$-ray energies is straightforward. The primary question that the experimenter must consider is the precision and accuracy to which he wishes to carry out such a measurement, and the corresponding care that must be taken.

In many cases it is adequate to represent the energy as a linear function of the channel, namely,

$$E(x) = a_1 + a_2 \cdot x$$  \hspace{1cm} (3.8)

where $x$ is the channel number and $E$ is the energy. It may even be adequate to determine the parameters $a_1$ and $a_2$ from only two well-chosen
values of $a_1$ and $a_2$. This method will distribute the deviations between the actual and computed energies more uniformly and also will reduce the sensitivity of the results to the particular choice of peaks and their location in the spectrum.

The pattern of the deviations from linearity for most of the curves in fig. 3.20 suggest that they would be reduced significantly if the energy were taken to be a quadratic function; that is,

$$E(x) = a_1 + a_2 \cdot x + a_3 \cdot x^2. \tag{3.10}$$

Although it is possible to compute the values of the parameters $a_1$, $a_2$, and $a_3$ from the energies and positions of only three peaks, they are usually determined by a least-squares fit to a set of more than 4 peaks. The input to such a fit includes the measured positions of the calibration peaks, their known energies and the uncertainties in these energies. (The peak positions also have uncertainties, but as discussed in section 1.6.1, these are usually ignored to simplify the fitting process.) The results of the least-squares fit are the values of $a_1$, $a_2$, and $a_3$ and their variances and covariances. For the data for curve a in fig. 3.20, the use of this function reduces the range of deviations from 0.111 keV for the linear function to 0.021 keV for the quadratic one.

The results of such a fit are sufficient to provide the energies and uncertainties for other $\gamma$-ray peaks in the same spectrum. The energy comes from eq. (3.10) and the variance in a $\gamma$-ray energy for a peak at channel $X \pm \sqrt{\text{var}(X)}$ is given by [see eq. (1.44) in section 1.5.3.3]

$$\text{var}(E) = \text{var}(X) \cdot (a_2 + 2 \cdot a_3 \cdot X)^2 + \text{var}(a_1) + \text{var}(a_2) \cdot X^2$$
$$+ \text{var}(a_3) \cdot X^4 + 2 \cdot \text{covar}(a_1, a_2) \cdot X$$
$$+ 2 \cdot \text{covar}(a_1, a_3) \cdot X^2 + 2 \cdot \text{covar}(a_2, a_3) \cdot X^3, \tag{3.11}$$

where the desired uncertainty is the square root of $\text{var}(E)$. In calculating the uncertainty of a $\gamma$-ray energy, the tendency will often be to truncate this uncertainty expression to a few terms or even just one. Of course, in some cases, such as when $\text{var}(X)$ is much larger than the corresponding variances of the calibration lines, the use of only the first term may be justified. But, it is preferable to evaluate the various contributions. It is expected that the contribution of the $\text{covar}(a_1, a_2)$ term will be negative so that the use of only the $\text{var}(a_i)$ terms will overestimate the uncertainty.

The quality of the fit to the calibration data can be judged from the $\chi^2$ value, which, as discussed in section 1.6.4, should be $\approx 1.0$. A significantly
smaller value probably indicates that the uncertainties assigned to the \(\gamma\)-ray calibration energies are too large. This can occur if these uncertainties include a large common contribution. In fact, the uncertainties used here should be those of the relative energies. Fortunately, one usually is not concerned with this distinction; however, for metrology measurements, care must be taken in this matter. On the other hand, if the \(\chi^2\) value is much greater than 1.0, it probably indicates that one of the assumptions of the least-squares fit does not hold; for example, the uncertainties assigned to the calibration energies are too small, one of the observed peaks does not represent the assigned \(\gamma\) ray or a more complex function is needed for \(E(x)\).

It should be emphasized the the magnitude of the deviations between the actual and computed energies for the expressions discussed above will often depend on how large a fraction of the channel range of the ADC is used. What is especially important is how low in the channel range the expression is applied. For example, the data in fig. 3.20 for the older system show that there can be large deviations from the parabola of eq. (3.10) below channel 400 of a 4096 channel ADC. Especially to handle this type of nonlinearity, Dryak (1986) suggests the alternative expressions

\[
E(x) = a \cdot x^{-1} + a_1 + a_2 \cdot x
\]  

(3.12a)

and

\[
E(x) = \beta \cdot x^{-2} + a \cdot x^{-1} + a_1 + a_2 \cdot x.
\]  

(3.12b)

In his test case, which includes 31 peaks from channel 59 to 3667, these expressions give much better fits than those in eqs. (3.8) and (3.10). Their usefulness depends on the form of the deviation from linearity at the lower channels.

Another method to deal with the nonlinearity of an ADC-amplifier system at the low-energy end was reported by Greenwood et al. (1970). They found it useful to simply measure the deviation from linearity of the electronic system and to apply this as a correction to the measured channel positions before the energy was calculated.

3.5 Energy measurements

3.5.1 Routine energy measurements

The discussion of the previous section has been in terms of an energy measurement in which the parameters of \(E(x)\) are determined from \(\gamma\)-ray peaks in the same spectrum as the lines for which the energies are to be calculated. For precise measurements this "internal" calibration is essential, and for routine measurements it is desirable.

However, in many situations, both in applications and in research, it is necessary to use an energy calibration that comes from a different spectrum. In a common situation, a calibration spectrum is measured once per day, and the resulting calibration is applied throughout the day. In many such cases the measured energies are only used to identify the nuclides and, thus, it is not necessary to quote any uncertainty on these values. However, if this is necessary, one should include an estimate of the effect of the change in calibration with time, count rate and room temperature.

Although a quantitative inclusion of these effects in the energies and uncertainties will generally not be possible, the experimenter should make an effort to determine their magnitude. As an indication of the possible magnitude of such variations in the calibration, table 3.8 gives the changes in the apparent energy of some peaks from a series of spectra for a source of \(^{152}\)Eu taken over a period of more than three weeks with no adjustment of the electronic system. For some spectra the count rate was increased as indicated by placing another source near the detector. For measurements
with only the $^{152}\text{Eu}$ source (≈ 3% dead time), the range of drift is 0.03 keV at 121 keV and 0.17 keV at 1408 keV. For the high-count-rate data, with a dead time of 20%, there is a zero shift of ≈ 0.05 keV. For any system whose drifts are this small, there will certainly be no problem with routine energy measurements without an internal calibration. These measurements were carried out in a temperature-controlled environment, and larger deviations would be expected if the temperature were to vary.

It is also possible to make use of a pulser to track the variation in the energy calibration with time and as environmental conditions change. For example, this can be done with a pulser that provides pulses of two, or more, very stable amplitudes. If the counts from the pulser pulses are stored with the γ-ray counts, the amplitudes of the pulser pulses need to be adjusted so that they do not coincide with any γ-ray peaks. It is more convenient if electronic routing can be used to store the pulser events in a

<table>
<thead>
<tr>
<th>Time</th>
<th>Analyzer Dead time (%)</th>
<th>Peak energies (keV)</th>
<th>Pulser-peak positions (channels)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>0.1</td>
<td>258.31</td>
<td>352.80(1) 3593.75(1)</td>
</tr>
<tr>
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<td>0.1</td>
<td>258.27(14)</td>
<td>352.81(1) 3593.74(1)</td>
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<td>258.56(12)</td>
<td>352.80(2) 3593.74(2)</td>
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<td>4.6</td>
<td>0.3</td>
<td>258.44(5)</td>
<td>352.80(2) 3593.76(2)</td>
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<tr>
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<td>14.0</td>
<td>258.56(1)</td>
<td>352.82(2) 3593.66(2)</td>
</tr>
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<td>35.0</td>
<td>258.43(1)</td>
<td>352.55(2) 3593.58(2)</td>
</tr>
<tr>
<td>8.7</td>
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</tr>
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</tr>
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</tr>
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<td>–</td>
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</tr>
<tr>
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<td>57.0</td>
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<td>352.71(2) 3593.53(2)</td>
</tr>
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<td>37.7</td>
<td>62.0</td>
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</tr>
<tr>
<td>Total spread</td>
<td>92</td>
<td>0.30</td>
<td>0.97</td>
</tr>
</tbody>
</table>

| Energy measurements |

3.5.2 Precise energy measurements

3.5.2.1 Experimental design

In the above discussion, the methodology of making γ-ray-energy measurements has been described. These methods are applicable to all measurements independent of the precision desired. However, for precise measurements there are additional considerations that need to be taken into account. As a guideline we might suggest that "precise" means obtaining an uncertainty of ≤ 10 eV at 100 keV and ≤ 30 eV at 1 MeV although uncertainties a factor of 10 smaller can be achieved. To make such measurements with Ge detectors, two methods are possible. First, one can determine the peak energy from the appropriate $E(\lambda)$ expression after a careful energy calibration. The second method involves the precise measurement of the energy difference between two closely spaced peaks. If the energy of one γ ray is well known, the other energy can be computed.
In the first case a large number of well-spaced calibration lines is needed in order to accurately determine all of the parameters in \(E(x)\). The calibration lines and the unknown lines of interest should all be well-resolved single peaks and must be measured at the same time. The desired \(\gamma\)-ray energies and their uncertainties follow from eqs. (3.10) and (3.11) or their equivalents if other expressions for \(E(x)\) are used. To reduce the statistical uncertainty of the final energy value, it is necessary that several measurements be made. It is possible that some local nonlinearity may exist in an ADC that can affect the result of any one measurement, or even a set of measurements if they are taken with the peaks at the same channels. Therefore, it is highly desirable that spectra be taken with the peaks at different channel locations (e.g., at slightly different gains). This procedure will provide some cancellation of any systematic error that is related to the local nonlinearity. Similarly, it is advantageous to make measurements on more than one detector system to gain change any systematic effect. If the detectors are of quite different sizes, some systematic effects such as the size of a Compton edge under a peak may be changed. A weighted average of the individual values should normally be used to obtain the final value.

There are two points in the treatment of such data where one must take care not to reduce, by averaging, an uncertainty contribution that is common to the various data values. As noted above the first occurs in the least-squares fit to determine the parameters of \(E(x)\) in which the uncertainty that is assigned to each calibration energy should not include any contribution that is common to the other calibration lines. One actually should use a correlation matrix for the weighting in such a fit since this allows one to take into account not only an uncertainty that is common to all the values, but also the relationships between any subset of the \(\gamma\)-ray energies. Since one seldom has the information and the capability to take the correlations into account, it is generally more expedient to remove any common factor before the fit and recombine it after the fit. (This is usually done by subtraction and addition in quadrature.) The second place where this is a concern is in the calculation of any average value, where any component of the uncertainties that is common to the values should be removed before the average is computed, and then recombined with the computed uncertainty.

In the second method for the determination of precise \(\gamma\)-ray energies, one measures the difference in energy between two closely spaced, but completely resolved, lines of which the energy of one is known. This method has three inherent advantages over that discussed above. First, it is often possible to use a set of calibration lines that cover a smaller portion of the spectral range, so \(E(x)\) will be a better approximation to the true energy–channel relation. Second, the measured energy difference is often very precise, many are known to 1 or 2 eV. Third, the energy difference is correct even if the energy of the known line of the pair changes significantly. This is true because the energy difference depends almost completely on the keV/channel ratio \(a_2\) term in eq. (3.10)) and very little on the energy of the nearest calibration line.

If the expression in eq. (3.10) is used for \(E(x)\), then the energy difference \(\Delta E = E_2 - E_1\) is given by

\[
\Delta E = a_2 \cdot \Delta X + a_3 \cdot \Delta (X^2)
\]

where \(\Delta X = X_2 - X_1\) is the difference in the centroids of the two \(\gamma\)-ray peaks and \(\Delta (X^2) = X_2^2 - X_1^2\). Then the variance of \(\Delta E\) is

\[
\text{var}(\Delta E) = a_2^2 \left[ \text{var}(X_2) + \text{var}(X_1) \right] + (\Delta X)^2 \cdot \text{var}(a_2) + \left[ \Delta (X^2) \right] \cdot \text{var}(a_3)
\]

\[
+ (2 \cdot a_3) \cdot \text{var}(X_1)
\]

\[
+ (2 \cdot a_3 \cdot X_2) - \text{var}(X_2) + 2 \cdot \Delta X \cdot \Delta (X^2) \cdot \text{covar}(a_2, a_3)
\]

\[
+ 2 (a_2 + 2 \cdot a_3 \cdot X_1) \cdot (a_2 + 2 \cdot a_3 \cdot X_2) \cdot \text{covar}(X_1, X_2)
\]

\[
+ 4 a_2 a_3 \left[ X_2 \cdot \text{var}(X_2) + X_1 \cdot \text{var}(X_1) \right].
\]

(3.13a)

If the two peaks are completely resolved, \(X_1\) and \(X_2\) are uncorrelated, so \(\text{covar}(X_1, X_2) = 0\), and if the contributions from \(a_3, [\Delta (X^2)]^2\) and \(\Delta X^2\) are all small

\[
\text{var}(\Delta E) = a_2^2 \left[ \text{var}(X_2) + \text{var}(X_1) \right].
\]

(3.14b)

As in the first method the measurement should be repeated several times with changes in the amplifier gain or another parameter to vary the peak positions. A weighted average of the individual values can be computed to obtain the final values of \(\Delta E\). If one wishes to obtain a very precise energy for the unknown \(\gamma\) ray, similar energy differences can be measured between it and other \(\gamma\) rays with known energies.

The work of Greenwood et al. (1979), in which over 100 energy differences are reported, is an example of the use of this method. Of the reported differences, 29 have uncertainties of only 1 or 2 eV. Even above 1 MeV, there are 24 differences with uncertainties of less than 5 eV. Other papers, as the \(^{152}\)Eu measurements of Warburton and Alburger (1966), have been published which give energy differences of similar quality along with the computed \(\gamma\)-ray energies.
3.5.2.2 Source-position effects

The nonlinearity of the electronics system certainly is the major influence on the choice of the $E(x)$ function. But, in addition, precise measurements of $\gamma$-ray energies require careful consideration of effects that occur in semiconductor detectors and can cause shifts in the observed peak positions. As discussed in section 2.1.6 these effects are called the "field-increment effect" for peak shifts produced by the acceleration of the electrons from the interaction of the $\gamma$ ray in the detector, and the "charge-collection effect" for any shift due to the nonuniform charge-collection properties. These processes produce variations in the pulse amplitudes that depend on the location of the event in the crystal and on the angle of incidence of the $\gamma$ rays. If all of the $\gamma$ rays come from one uniform source, this is not a problem. However, when sources in different measuring geometries are used (e.g., the source of the unknown lines and that of the energy-calibration lines are at quite different distances), one has the potential for shifts in the relative peak positions, so that slightly different $E(x)$ functions would apply for the different geometries.

There have been several measurements of the shift in the apparent $\gamma$-ray energy between sources in front of and beside a planar detector. As illustrated in fig. 3.21, this shift may be 50 eV for a full-energy peak at 1 MeV, and 300 eV at 3 MeV. These results, which are from Helmer et al. (1975b), agree well with those of Gunnink et al. (1968), Heath (1969) and Shizuma et al. (1978).

As discussed in section 2.1.6, the comparable shift for double-escape peaks is expected to be much smaller than that for the full-energy peaks; this is confirmed by the results shown in fig. 3.21. The difference in the sign of the shift for the full-energy and double-escape peaks may result from a somewhat longer mean path length for the positrons from the pair production. If one considers the use of both double-escape and full-energy peaks...
in any energy measurement, this relative shift needs to be taken into account. With a planar detector, this might be done by having all of the γ rays enter the detector perpendicular to the electric field.

So far we have only compared sources whose γ rays entered the detector from very different directions. However, as discussed in section 2.1.6, even for sources at the same angle, but different distances, there is a contribution from these effects. This is illustrated in fig. 3.22. Although we have only discussed these observed results for planar detectors in terms of the field-increment effect, they include some contribution from the nonuniformity in the charge collection.

For coaxial detectors the situation will be more complex and the net effect may depend on the relative magnitudes of the charge-collection and field-increment contributions. This means the effect may vary considerably between detectors. As an indication of the magnitude of the observed effects, and their variation between detectors, fig. 3.22 shows the shift in the apparent energy of the 1489 keV γ rays as a function of the source–detector distance for a planar, an open-end coaxial, and four closed-end coaxial detectors. It is interesting to note that the closed-end coaxial detectors give quite different results - two with positive shifts, one with a negative shift and the last with essentially no shift. As expected, the open-end coaxial detector has essentially no shift because the γ rays enter the detector perpendicular to the electric field. However, in contrast to this result large shifts have been reported by others for open-end coaxial detectors. Roehmer (1972) has reported a large shift of about 240 eV at 1300 keV between source–detector distances of 1.25 and 36.8 cm compared to less than 15 eV in our case, and Inoue et al. (1973) have reported a shift of about 55 eV at 1275 keV between 2 and 35 cm. Further results are reported by Lichtenberger and MacKenzie (1974), Sakai and Katagiri (1977), and Shizuma et al. (1978).

3.5.2.3 Decay-scheme fitting

So far the discussion in this section has been concerned with the measurement techniques, but there is one widely used analytical method that should be described. With the use of Ge detectors, it has become feasible to measure many of the γ-ray energies of a complex decay scheme. Especially interesting examples of this are the decay of $^{187}$Ta and $^{190}$Ag$^{m}$. Once the majority of the energies within a scheme have been measured, it can be quite useful to determine the most precise and most consistent set of level energies from a least-squares fit, and then use these level energies to compute a set of consistent γ-ray energies. The computed γ-ray energies may include all the γ rays in the decay scheme, not just those measured.

For such a fit, the common component of the uncertainty, in particular the uncertainty in the energy scale, should be removed before the calculation and then recombed afterwards. This least-squares analysis can also be designed to make direct use of any energy differences measured between γ rays within this level scheme. This fact can be especially useful in the two decay schemes noted above because they have a number of closely spaced γ rays. Examples of this level-energy-fitting technique can be found in the work of Warburton and Alburger (1986), Helmer et al. (1978), and Greenwood et al. (1979). A variation of this method was used by Kennett et al. (1983) to obtain the energies of the γ lines from several reactions including $^{14}$N($n, \gamma$)$^{15}$N (see fig. 1.13). In this case the energy calibration itself was done by determining the parameters of the $E(x)$ expression that best fit both the level scheme constraints for the cascade–crossover combinations and the 511-keV energy differences between the full-energy, single-escape, and double-escape peak energies.
References

Baerg, A.P., 1966, Metrologia 2, 23.
Bambeynek, W., 1984b, Internal Report GE-R-RN-18-84 (Central Bureau of Nuclear Measurements, Geel, Belgium).
Bambeynek, W., 1987, private communication.