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Date: 2023-06-18T00:00:00+00:00

Abstract

Based on the statistical characteristics of energy spectrum and the features of spectrum-shifting in spectrometry, the parameter adjustment method of Gaussian function space was applied in the simulation of spectrum-shifting. The transient characteristics of energy spectrum were described by the Gaussian function space, and then the Gaussian function space was transferred by parameter adjustment method. Furthermore, the spectrum-shifting in measurement of energy spectrum was simulated. The applied example shows that the parameters can be adjusted flexibly by this method to meet the various requirements in simulation of energy spectrum-shifting. This method was one parameterized simulation method with good performance for the practical application.

Full Text

Preamble

Simulation of γ Spectrum-Shifting Based on Parameter Adjustment of Gaussian Function Space

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Abstract: Based on the statistical characteristics of energy spectra and the features of spectrum-shifting in spectrometry, we applied a parameter adjustment

method for Gaussian function space to simulate spectrum-shifting. The transient characteristics of energy spectra were described using Gaussian function space, which was then transformed through parameter adjustment to simulate spectrum-shifting in energy spectrum measurement. An applied example demonstrates that this method allows flexible parameter adjustment to meet various requirements in simulating energy spectrum-shifting. This parameterized simulation method exhibits good performance for practical applications.

Key words: Gaussian function space, parameter adjustment, simulation of energy spectrum-shifting

Introduction

In radioactivity measurement, spectrum-shifting commonly occurs due to various factors. This paper combines the statistical characteristics of energy spectra with the features of spectrum-shifting and presents a simulation method for gamma spectrum-shifting based on parameter adjustment of Gaussian function space.

2 Gaussian Function Space

The Gaussian function space is constructed using multiple Gaussian basis functions. Consider a Gaussian function Φ(t) defined as:

$$\Phi(t) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{t^2}{2\sigma^2}}$$

where σ is the standard variance and k is the translation value. Its integer translation function can be expressed as Φ(t-k). The telescopic translation function of Φ(t) is Φjk(t), given by:

$$\Phi_{jk}(t) = 2^{j/2}\Phi(2^{jt} - k), \quad j, k \in \mathbb{Z}$$

where j represents the scaling factor. The following inner product can be acquired:

$$\langle \Phi_{jk}(t), \Phi_{jk'}(t) \rangle = \int \Phi_{jk}(t)\Phi_{jk'}(t)dt$$

When σ takes the minimum value, $\langle \Phi_{jk}(t), \Phi_{jk'}(t) \rangle$ (k≠k) approaches zero. For example, when σ=0.15, the result of $\langle \Phi_{0k}(t), \Phi_{0k'}(t) \rangle$ (k≠k) is on the order of 10^{-5}; when σ=0.1, it is on the order of 10^{-11}, which can be regarded as zero. Additionally, it is easy to verify that $\langle \Phi_{0k}(t), \Phi_{0k}(t) \rangle = 1$ from the formula above. The following relationship can be established:

$$\langle \Phi_{jk}(t), \Phi_{jk'}(t) \rangle = \delta(k - k')$$

where δ(k-k) = 0 (k≠k) and δ(k-k) = 1 (k=k). Therefore, when σ takes the minimum value, Φjk(t) exhibits orthogonality. The space V_j = span$\{\Phi_{jk}(t)\}$ (j,k) formed by Φjk(t) can be regarded as the Gaussian function space, with Φjk(t) serving as the orthogonal basis in space Vj. Using $P_{jf}(t)$ to represent the projection of f(t) in the Gaussian function space Vj:

$$P_{jf}(t) = \sum_k \langle f(t), \Phi_{jk}(t) \rangle \Phi_{jk}(t)$$

3 Expression of γ Energy Spectrum Using Gaussian Function Space

Multiple small Gaussian functions can effectively approximate and simulate radioactive energy spectra, and multi-scale analysis can extract signal characteristics efficiently. The short transient characteristics of energy spectra can be described using Gaussian function space, and parameter adjustment for the state transition of Gaussian function space, combined with the statistical fluctuation characteristics of energy spectra, can simulate spectrum-shifting in energy spectrum measurement. In fact, the projection of an energy spectrum onto the function space Vj composed of Gaussian functions is expressed linearly by multiple Gaussian functions, where each Gaussian function affects the count of all channels through its weight. Consequently, the count of any channel is influenced by adjacent channels, with closer channels exerting greater influence. This method aligns with the statistical characteristics of actual spectra.

For γ energy spectra specifically, the representation using Gaussian function space can be expressed in detail as follows. Assume the original energy spectrum is f(n) (n=1…N), where N is the total number of channels and the gross count is Ntotal. The spectrum can be represented using Gaussian functions through the following steps:

First, regard f(n) as a continuous function f(t) and choose a Gaussian function space Vj (typically with j$ $0). The projection of f(t) in Vj is given by $P_{jf}(t)$. If f(t) Vj, the signal can be further expressed using basis functions in space Vj as:

$$f(t) = \sum_k c_{jk} \Phi_{jk}(t)$$

According to the projection formula, $c_{jk} = \langle f(t), \Phi_{jk}(t) \rangle$. For convenience, this can be expressed as:

$$c_{jk} = \sum_{n=1}^{N} f(n)\Phi_{jk}(n)$$

where cjk represents the weight of the linear combination. In radioactivity measurement, the energy spectrum signal f(n) can be regarded as the discrete form of some function f(t) V0. Parameter λ is the same as in the telescopic translation function formula, and f(2^- k) can take the average of the local area where t=2^- k. In actual calculation, Φjk(t) can take several or dozens of discrete values in the local area where t=2^- k, which greatly reduces the computational amount.

The final energy spectrum f (n) can be obtained through rounding and discretization according to the following formula:

$$f'(n) = \text{round}\left(\frac{N_{\text{total}} \cdot P_{jf}(n)}{\sum_{n=1}^{N} P_{jf}(n)}\right)$$

Formula (12) can be regarded as a correction for the non-orthogonality of the Gaussian function space. The f (n) obtained according to formula (12) is exactly the space expression of the energy spectrum. Random numbers will be generated to simulate the energy spectrum shift and statistical fluctuation process. The generation of random numbers can employ either random sampling methods of the Gaussian mixture function or discrete direct sampling methods.

Simulation of γ Spectrum-Shift Within Gaussian Function Space

4.1 Random Sampling of Gaussian Mixture Function

The original energy spectrum can be decomposed into combinations of uniform distribution, Gaussian distribution, exponential distribution, and polynomial distribution, which enables effective simulation of nuclear energy spectra. As shown in the preceding analysis, peak position shift frequently occurs in energy spectrum measurement. Therefore, further research to solve the simulation problem of peak position shift is necessary. If energy spectrum shift can be simulated effectively, it would undoubtedly be of great significance to energy spectrum studies.

Peak position shift may be caused by many factors, but a generally applicable model is expressed in Fig. 1 [Figure 1: see original paper]. The gamma ray excitation signal is determined by the radioactive nuclide. Observable parameters of the Gaussian function space are very sensitive to external environment and test conditions, such as temperature, counting rate, high voltage changes, and other factors.

The principle of using Gaussian function space to simulate gamma energy spectrum shift is as follows: a Gaussian function space describes the instantaneous or short-term gamma spectrum, and its parameters (e.g., mean, standard variance) are adjusted over time according to patterns that simulate external environment and test conditions, such as changing temperature, varying counting rates, changing high pressure, and other factors. Finally, random sampling generates the shifted spectrum.

The random sampling of the Gaussian mixture function was realized using the additive sampling method. First, normalize the energy spectrum in Gaussian function space into the following form:

$$\rho(x) = \sum_{n=1}^{M} P_n f_n(x)$$

where $P_n \geq 0$, $\sum_{n=1}^{M} P_n = 1$ (n=1…M), $f_n(x)$ is a Gaussian density function related to parameter n (n=1,2,…M), and M is the number of Gaussian density functions. Second, determine n through random sampling and obtain the random number (x) by random sampling according to function $f_n(x)$.

4.2 Discrete Direct Sampling Method

First, normalize the energy spectrum in Gaussian function space into a density function (x). The discrete distribution function F(x) is given by:

$$F(x) = \sum_{i=1}^{I} \rho(x_i)$$

where x_i is the discrete point of the density function (x), which corresponds to the channel number of the energy spectrum, (xi) is the corresponding probability, and $\sum_{i=1}^{N} \rho(x_i) = 1$ (I=1…N). With the random number x calculated according to:

$$x = x_{I-1} + \frac{\epsilon - F(x_{I-1})}{\rho(x_I)}$$

simulation of the F(x) distribution on the energy spectrum can be obtained, where is a random number from a uniform distribution within [0, 1]. The resulting x_I is precisely the random number x_F of the distribution function F(x).

4.3 Example Analysis

Using the model shown in Fig. 1, the shift of the ^{40}K γ spectrum represented by $S_1(\cdot)$ in Fig. 2 can be simulated. The γ spectrum was measured

by a 1024-channel NaI(Tl) scintillation spectrometer with a gross count of 1.9247$×10^{5}$ (Ntotal=1.9247$×10^{5}).*TheselectedGaussianfunctionspaceisV*_{3}$, which contains 128 Gaussian functions with standard variance σ=1. The ^{40}K γ spectrum curve in the Gaussian function space is shown as S_2(-) in Fig. 2.

Since channels are integers, the final energy spectrum must be obtained after rounding operations on the sampled channels from the Gaussian function space. Figure 3 [Figure 3: see original paper] shows the shift process of the entire energy spectrum. The dashed lines (–) represent the energy spectra at different times during measurement, shifting from left to right, where shorter times correspond to lower curves. The solid line (-) represents the energy spectrum after shifting by 40 channels, with a gross count of 1.9247$×10^{5}$. Figure 4 [Figure 4: see original paper] shows the final energy spectra with and without shifting.

For simplicity, only steady spectrum shift to the right (i.e., energy spectrum shifting at constant speed toward higher energy) was simulated; the method for leftward shift is similar. In practice, the transfer process of Gaussian function space can be designed in linear or non-linear modes to simulate complex spectrum shifts caused by temperature and humidity influences.

Assuming the number of shift channels is 40, the continuous shift process can be discretized into 80 Gaussian function spaces, meaning the interval between two adjacent Gaussian function spaces is 0.5 channel. In fact, intervals can be set to 0.1, 0.2, 0.3, ..., 1, 1.1, 1.2, etc. The smaller the interval, the more accurately the shift process can be achieved, which represents a main advantage of this method. Additionally, because channels are integers, rounding is necessary.

Figure 5 [Figure 5: see original paper] shows the statistical fluctuation process simulated by generating random numbers to model energy spectrum shift with a peak position shift of 40 channels to the right. This example clearly demonstrates that Gaussian function space can conveniently, realistically, and visually simulate gamma energy spectrum shift as a state transition method. Moreover, the model can easily simulate the fluctuation process of energy spectra when measurement environments or conditions change, such as detector resolution, external temperature, and humidity. The state transition of Gaussian function space is accomplished through parameter adjustment of the Gaussian functions, such as mean value adjustment and standard variance adjustment.

This article presents only a simulation example of spectrum shift toward higher energy; the method for shift toward lower energy is similar. Parameters can be flexibly adjusted to satisfy diverse simulation requirements for spectrum shift. For instance, the transition state can be designed as linear or non-linear functions to simulate spectrum shifts in complex environments, the number of Gaussian function spaces can be increased to simulate slow spectrum shifts, and parameter j (j = 0, 1, 2, 3...) in the telescopic translation function can be used to increase or decrease the dimension of Gaussian function space to improve energy spectrum accuracy, enhance statistical fluctuation suppression capability, and increase computing speed.

Table 1 and Fig. 6 compare the theoretical spectrum peak with the sampling spectrum peak after shifting. The two curves in Fig. 6 almost coincide, with most channel errors ranging from 0.07% to 2% as shown in Table 1, indicating that this method is practicable. Note that the gross count was increased to Ntotal=1.9247$×10^{6}$ to improve simulation accuracy.

In energy spectrum measurement, γ-ray spectrum-shifting usually occurs when conditions such as high voltage, temperature, or count rate change, and the forms of shift vary widely. However, with our proposed method, random nuclear signals that meet the demands of diversity, flexibility, variability, and repeatability under complex conditions can be easily generated to simulate spectrum-shifting. This is because these conditions can be described collectively, rather than individually, through the state transition of Gaussian function space. In digital nuclear instrument and algorithm research, spectrum-shifting is typically considered under all conditions rather than a single condition. In fact, studying spectrum-shifting under a special condition is unnecessary. Therefore, random nuclear signals generated by this method can meet the demands of spectrum-shifting processing in digital nuclear instrument and algorithm research, and can improve instrument performance.

5 Conclusion

This article proposes an approach that combines the statistical characteristics of energy spectra with the features of spectrum-shifting in radioactivity measurement, presenting a simulation method for gamma spectrum-shifting based on parameter adjustment of Gaussian function space. Spectrum-shifting in energy spectrum measurement can be simulated through the description of short transient characteristics of energy spectra in Gaussian function space and parameter adjustment for state transition of Gaussian function space. The examples demonstrate that parameters can be flexibly adjusted to satisfy diverse simulation requirements for spectrum shift. This parameterized simulation method exhibits good performance in practical applications.

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Note: Figure translations are in progress. See original paper for figures.