Simulation of γ spectrum-shifting based on the parameter adjustment of Gaussian function space

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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.

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

1 Introduction

Nuclear signal generator and relevant generation method are one of the most important tools in the research of digital nuclear instruments. Using nuclear signal that meets the demand of diversity, flexibility, variability and repeatability can verify the performance of the digital nuclear instrument directly. In the measurement of energy spectrum, the peak position shift problems occur usually. Such as the magnification of photomultiplier tube and its spectral response, the photon yield of scintillator (for the fixed energy rays) changes with temperature, which will cause the output pulse amplitude of detector change and the peak position shift. In addition, the magnification of linear pulse amplifier that changes with temperature will cause peak position shift. Furthermore, the magnification of photomultiplier in detector will be influenced by the changes of count rate and high pressure, which will also cause the peak position shift[1,2]. This article combines the statistical characteristics of energy spectrum with the features of spectrum-shifting in the radioactivity measurement, and then gives the simulation method of gamma spectrum-shifting based on the parameter adjustment of Gaussian function space.

2 Gaussian function space

The Gaussian function space is constructured by multiple Gaussian basis functions[3–7].

Assume a Gaussian function as Φ(t), Φ(t) is given as

$$\varphi(t)=\frac{1}{\sqrt{2\pi}\sigma\lambda}\exp[-\frac{1}{2\sigma^2}t^2] \tag{1}$$

Its integer translation function can be expressed as

$$\varphi_{0k}(t)=\frac{1}{\sqrt{2\pi}\sigma\lambda}\exp[-\frac{1}{2\sigma^2}(t-k)^2]\ ,\ k\in Z \tag{2}$$

where

$$\lambda=\sqrt{\int_{-\infty}^{+\infty}\{\frac{1}{\sqrt{2\pi}\sigma}\exp[-\frac{1}{2\sigma^2}t^2]\}^2\mathrm{d}t}\ ,$$

σ is the standard variance, and k is translation value.

Assume the telescopic translation function of $\Phi(t)$ is $\Phi_{jk}(t)$, $\Phi_{jk}(t)$ is given as

$$\phi_{jk}(t)=2^{\frac{-j}{2}}\phi(2^{-j}t-k)(j,k\in Z) \tag{3}$$

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And

$$\varphi_{jk}(t)=2^{-0.5j}\frac{1}{\sqrt{2\pi}\sigma\lambda}\exp[-\frac{1}{2\sigma^2}(2^{-j}t-k)^2] \qquad (4)$$

where j is the telescopic size.

The following inner product can be acquired.

$$\begin{aligned}&\langle\phi_{(j+1)k}(t),\phi_{(j+1)k'}(t)\rangle=\int 2^{\frac{-(j+1)}{2}}\phi(2^{-(j+1)}t-k)2^{\frac{-(j+1)}{2}}\phi(2^{-(j+1)}t-k')dt\\&=\frac{1}{2}\int 2^{\frac{-j}{2}}\phi(\frac{2^{-j}}{2}t-k)2^{\frac{-j}{2}}\phi(\frac{2^{-j}}{2}t-k')dt\\&=\int 2^{\frac{-j}{2}}\phi(2^{-j}t'-k)2^{\frac{-j}{2}}\phi(2^{-j}t'-k')dt' \quad (t'=\frac{t}{2})\\&=\int\phi_{jk}(t')\phi_{jk'}(t')dt'=\langle\phi_{jk}(t'),\phi_{jk'}(t')\rangle\end{aligned}$$

…(5)

When σ takes the minimum value, $<\Phi_{jk}(t), \Phi_{jk'}(t)>$ ($k\neq k'$) is near zero, for example, when σ=0.15, the consequence of $<\Phi_{0k}(t), \Phi_{0k'}(t)>(k\neq k')$ is the order of magnitude of 10^{-5}, when σ=0.1, the consequence of $<\Phi_{0k}(t), \Phi_{0k'}(t)>(k\neq k')$ is the order of magnitude of 10^{-11}, which can be regarded as zero.

In addition, it is easy to get that $<\Phi_{0k}(t), \Phi_{0k}(t)>$ =1 from formula (2). The following relationship can be established by formula (5).

$$<\phi_{jk}(t)\phi_{jk'}(t)>=\sigma(k-k') \qquad (6)$$

where $\delta(k-k')=0$ ($k\neq k'$), $\delta(k-k')=1$($k=k'$). So, it can be considered that when σ take the minimum value, $\Phi_{jk}(t)$ has the orthogonality relationship. The space V_j= $span\{\Phi_{jk}(t)\}(j,k\in Z)$, which formed from $\Phi_{jk}(t)$, can be regarded as the Gaussian function space and then $\Phi_{jk}(t)$ can be regard as the orthogonal basis in space V_j .

Using $P_jf(t)$ to present the projection of $f(t)$ in the Gaussian function space V_j:

$$p_jf(t)=\sum_{k=-\infty}^{+\infty}c_{jk}\phi_{jk}(t) \qquad (7)$$

If $f(t)\in V_j$, signal $f(t)$ can be expressed further with basic functions in space V_j as follow:

$$f(t)=p_jf(t)=\sum_{k=-\infty}^{+\infty}c_{jk}\phi_{jk}(t) \qquad (8)$$

where c_{jk} is the weight of linear combination, and is given by

$$c_{jk}=<f(t),\phi_{jk}(t)> \qquad (9)$$

In radioactivity measurement, energy spectrum signal $f(n)$ can be regarded as the discrete form of some function like $f(t)\in V_0$.

3 The expression of the γ energy spectrum by Gaussian function space

Multiple small Gaussian functions can be used to get the good approximation and simulation of radioactive energy spectrum[8,9], and the multi-scale analysis can extract characteristics of signal effectively[10,11]. The short transient characteristics of energy spectrum can be described by using Gaussian function space, and the parameter adjustment for the state transition of Gaussian function space combined with statistical fluctuation characteristics of energy spectrum can be employed to simulate the spectrum-shifting in energy spectrum measurement. In fact, the projection of energy spectrum on the function space V_j made up of Gaussian functions is expressed linearly by multiple Gaussian functions, and each Gaussian function can affect the count of all channels by its weight, namely the count of any channel will be affected by adjacent channels, moreover, the more adjacent channel has, the greater effect it will cause. This method is accord with the statistical characteristics of actual spectrum.

Take the example of γ energy spectra, the representation of Gaussian function space can be expressed in details as below.

Assume the original energy spectrum is $f(n)$ (n=1…N), where N is the total number of channels, and the gross count is N_{total}. Using Gaussian function to show it in following steps:

Regard the original spectrum $f(n)$ as a continuous function $f(t)$, and choose a Gaussian function space V_j, which is chosen as $j\geq 0$ usually, then the projection of $f(t)$ in the V_j is given by

$$p_jf(t)=\sum_{k=1}^{N/2^j}c_{jk}\phi_{jk}(t) \qquad (10)$$

According to formula (9), c_{jk}= $<f(t), \Phi_{jk}(t)>$, for convenience, it can be expressed as

$$\begin{aligned}c_{jk}&=<f(t),\varphi_{jk}(t)>\\&\approx f(2^jt)\int_{-\infty}^{+\infty}\varphi_{jk}(t)\mathrm{d}t\\&=2^{\frac{j}{2}}f(2^jk)/\lambda\end{aligned} \qquad (11)$$

Parameter λ is the same as the λ in formula (2), $f(2^jk)$ can take the average of local area where t=2^jk. In the

actual calculation, $\Phi_{jk}(t)$ can take several or dozens of discrete values at local area where $t=2^j k$, which will reduce the calculation amount of formula (10) greatly.

The final energy spectrum $f'(n)$ can be obtained according to the rounding and discretization of following formula.

$$f'(n) = N_{\text{total}} P_j f(n) / \sum_{n=1}^{N} P_j f(n), \ (n = 1 \cdots N) \quad (12)$$

Formula(12) can be regarded as the revised formula for the nonorthogonality of Gaussian function space, $f'(n)$ according to formula (12) is exactly the space expression of energy spectrum.

4 Simulation of γ spectrum-shift within the Gaussian function space

The original energy spectrum can be decomposed to the combination of uniform distribution, Gaussian distribution, exponential distribution and polynomial distribution, which can be used to the effective simulation of nuclear energy spectrum[6]. Primitive preceding analysis shows that the peak position shift often happens in the energy spectrum measurement. Therefore, in order to solve the simulation problem of peak position shift, the further research is very necessary. If the shift of the energy spectrum can be simulated by effective methods, undoubtedly, it is of great significance to the study of energy spectrum. Peak position shift may be caused by many factors, but the generally available model is expressed as in Fig.1.

The gamma ray excitation signal is determined by the radioactive nuclide. Observable parameters of the Gaussian function space are very sensitive to the external environment and test conditions, such as the temperature, the counting rate, the change of high voltage and other factors.

The principle of Gaussian function space to simulate the gamma energy spectrum shift is: using a Gaussian function space to describe the instantaneous or short time gamma spectrum; Gaussian function space parameters (e.g., mean, standard variance) will be adjusted over time, which has the adjustment pattern made of requirements to simulate the external environment and test conditions, such as the changing temperature, the diverse counting rate, the changing high pressure and other factors. Finally, the random numbers will be generated to simulate energy spectrum shift and statistical fluctuation process. The generation of random numbers can take random sampling method of the Gaussian mixture function or discrete direct sampling method.

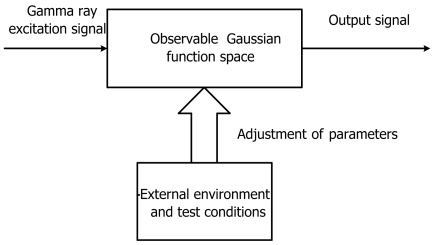

Fig.1 Model of γ spectrum-shifting.

4.1 The random sampling of Gaussian mixture function.

The random sampling of Gaussian mixture function was realized by the additive sampling method[12,13]. first of all, normalize the energy spectrum in Gaussian function space into the form of following formula

$$f(x) = \sum_{n=1}^{M} P_n f_n(x) \quad (13)$$

where, $P_n \geq 0$, $\sum P_n = 1 (n = 1 \ldots M)$, $f_n(x)$ is a Gaussian density function which is related to parameter $n (n = 1,2,\ldots M)$, and M is the number of Gaussian density functions. Secondly, determine n by random sampling to get the random number (x) by random sampling according to function $f_n(x)$.

4.2 Discrete direct sampling method

Firstly, normalize the energy spectrum in Gaussian function space into a density function $\rho(x)$, the discrete distribution function of $F(x)$ is given as

$$F(x) = \sum_{x_i < x} \rho(x) \quad (14)$$

where x_i is the discrete point of density function $\rho(x)$, that is also the serial number of the channel of energy spectrum, $\rho(x_i)$ is the corresponding probability, and $\sum \rho(x_i)=1$ $(I=1 \ldots N)$. With the random number x calculated according to the sampling of (15), simulation of $F(x)$ distribution on energy spectrum can be obtained, ε is the random number of uniform distribution within [0, 1][14,15].

$$x_F = x_I, \ when \sum_{i=1}^{I-1} \rho(x_i) \le \varepsilon < \sum_{i=1}^{I} \rho(x_i) \qquad (15)$$

where x_I is just the random number x_F of distribution function $F(x)$.

4.3 Example analysis

With the model shown in Fig.1, the shift of ^{40}K γ spectrum shown by $S_1(.)$ in Fig.2 can be simulated. The γ spectrum is measured by the 1024-channel NaI (Tl) scintillation spectrometer, with the gross count of 1.9247×10^5, namely $N_{total}=1.9247\times10^5$. The selected Gaussian function space is V_3, which has 128 Gaussian functions, and has the standard variance σ (σ=1).The ^{40}K γ spectrum curve in the Gaussian function space is shown by S_2(-) in Fig.2.

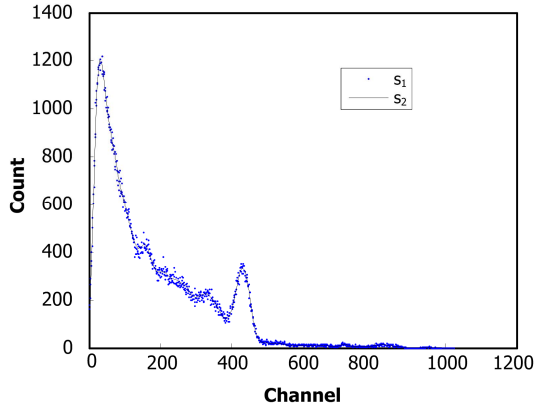

Fig.2 Original γ spectrum(·) and γ spectrum in Gaussian function space(—) of ^{40}K.

For simplicity, only the steady spectrum shift to the right (that is, the energy spectrum shift at a constant speed and in the direction of high energy) was simulated, the simulation method of shift to left is similar. Actually, the transfer process of Gaussian function space can be designed as linear or non-linear mode to simulate the complex spectrum shift by the influence of temperature and humidity.

Assumed the number of shift channels is 40, then the continuous shift process can be dispersed into 80 Gaussian function spaces, namely, the interval between the two adjacent Gaussian function spaces is 0.5 channel. In fact, interval can get 0.1, 0.2, 0.3, ..., 1, 1.1, 1.2, etc., the smaller the interval is, the more accurate the shift process of energy spectrum can achieve, which is also the main advantage of this method. In addition, because the channel is an integer, so it must get the integer energy spectrum after rounding operation on the sampled channels of Gaussian function space finally.

Figure 3 shows the shift process of the entire energy spectrum. The dashed line(--) represents each entire energy spectrum in different time in the spectrum measurement, shifting from left to right, the shorter the time is，the lower the curve is. The solid line(-) represents the entire energy spectrum after shifting for 40 channels, with a gross count of 1.9247×10^5. Figure 4 shows the ultimate energy spectrum without shifting, and one with shifting.

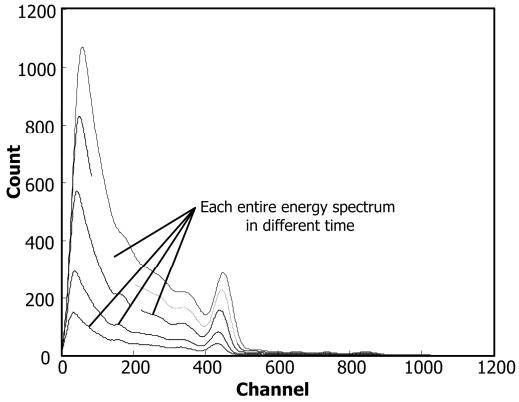

Fig.3 Shift process of entire spectrum in Gaussian function spaces.

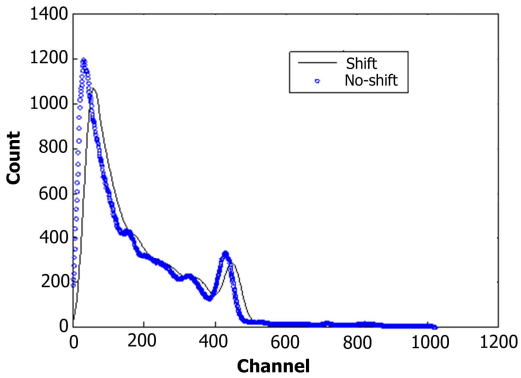

Fig.4 Shifting spectrum (—) and no-shifting spectrum (o).

Figure 5 shows the statistical fluctuation process by generating random numbers to simulate energy spectrum shift, which has peak position shift to the right way for 40 channels. From this example, it is clear that the Gaussian function space can be used to simulate the gamma energy spectrum shift as a state transition method conveniently, realistically and visually. In addition, the model can be easily used to simulate the fluctuation process of energy spectrum

when measuring environment or condition, such as detector resolution, external temperature and humidity, changes. Actually, the state transition of Gaussian function space is completed by parameter adjustment of the Gaussian function, such as mean value adjustment and standard variance adjustment.

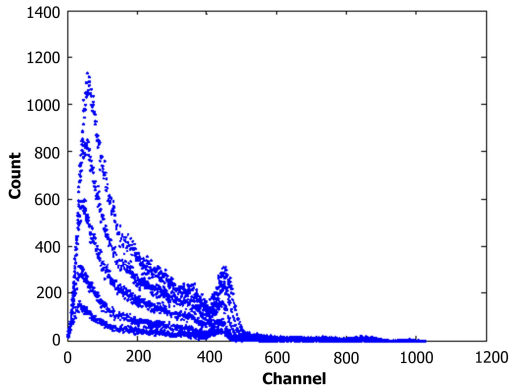

Fig.5 Simulation of statistical fluctuation process for γ spectrum-shifting.

This article only gives a simulation instance of spectrum shift in the direction of high energy. The simulation method of spectrum shift in the direction of low energy is similar.

The parameters can be flexibly adjusted to satisfy the requirements of the diversity for the simulation of spectrum shift. For example, the transition state can be designed as linear or non-linear function to simulate the spectrum shift in a complex environment, the number of Gaussian function spaces can be increased to simulate the spectrum shift with slow speed, and the parameter j (j = 0, 1, 2, 3...) in formula (3) can be used to increase or decrease the dimension of Gaussian function space in order to improve the accuracy of the energy spectrum, or improve the ability of inhibiting statistical fluctuation and increase computing speed.

Comparison of theoretical spectrum peak and sampling spectrum peak after shifting is showed in Table 1 and Fig.6. Two curves in Fig.6 almost coincide with each other, and most of errors in these channels are 0.07%–2%, as showed in Table 1, indicating that this method is practicable. Where, the gross count is increased to N_{total}=1.9247×10^6 in order to improve the simulating accuracy of the energy spectrum.

In the energy spectrum measurement, γ-ray spectrum-shifting occurs usually when the conditions change, such as the high voltage, temperature, count rate, etc, and the forms of shift are very different. However, with our proposed method, random nuclear signals, which meet the demand of diversity, flexibility, variability and repeatability under complex conditions, can be easily generated to simulate the spectrum -shifting, because these conditions can be described collectively, not respectively, by the state transition of Gaussian function space. In the course of studying on the digital nuclear instrument and algorithm, the spectrum- shifting is usually considered under all conditions, not one condition. In fact, it is not necessary and impractical to measure the spectrum-shifting under a special condition. Therefore, random nuclear signals generated by this method can meet the demand of spectrum-shifting processing in the studying on the digital nuclear instrument and algorithm, and this method can improve the performance of instrument.

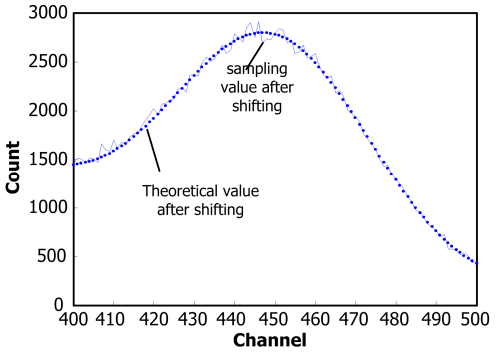

Fig.6 Comparison of theoretical spectrum peak and sampling spectrum peak after shifting. solid line(-): sampling value of spectrum after shifting; dashed line(··): theoretical value of spectrum after shifting.

5 Conclusion

This article proposed an approach that combines the statistical characteristics of energy spectrum with the features of spectrum-shifting in the radioactivity measurement, and gives the simulation method of gamma spectrum-shifting based on the parameter adjustment of Gaussian function space. The spectrum-shifting in energy spectrum measurement can be simulated by the description of short transient characteristics of energy spectrum in Gaussian function space, and the parameter adjustment for the state transition of Gaussian function space.

The instances show that, by this method, the parameters can be flexibly adjusted to satisfy the

requirements of the diversity for the simulation of spectrum shift. The parameterized simulation method has a good performance in actual application.

Table 1 Comparison of theoretical spectrum peak and sampling spectrum peak after shifting

Ch	Theo-val	Samp-val	Error (%)	Ch	Theo-val	Samp-val	Error (%)	Ch	Theo-val	Samp-val	Error (%)	Ch	Theo-val	Samp-val	Error (%)	Ch	Theo-val	Samp-val	Error (%)
400	1445	1464	1.3	420	1920	2021	5.26	440	2707	2789	3.03	460	2488	2579	3.66	480	1283	1287	0.31
401	1450	1511	4.2	421	1961	1949	–0.61	441	2730	2752	0.81	461	2442	2463	0.86	481	1223	1245	1.8
402	1456	1508	3.6	422	2004	2067	3.14	442	2749	2695	–1.96	462	2392	2367	–1.05	482	1164	1185	1.8
403	1465	1469	0.27	423	2047	2077	1.47	443	2765	2849	3.04	463	2340	2330	–0.42	483	1107	1099	–0.72
404	1476	1517	2.8	424	2091	2107	0.77	444	2778	2897	4.28	464	2286	2352	2.89	484	1051	1059	0.76
405	1489	1510	1.4	425	2136	2115	–0.98	445	2787	2746	–1.47	465	2229	2178	–2.29	485	997	972	–2.51
406	1504	1467	–2.5	426	2180	2215	1.6	446	2793	2911	4.22	466	2171	2209	1.75	486	945	955	1.06
407	1521	1658	9	427	2224	2234	0.45	447	2795	2688	–3.83	467	2111	2150	1.85	487	895	886	–1.01
408	1540	1601	4	428	2269	2186	–3.66	448	2793	2735	–2.08	468	2050	2003	–2.29	488	847	833	–1.65
409	1561	1587	1.7	429	2313	2364	2.2	449	2788	2727	–2.19	469	1987	1969	–0.91	489	800	798	–0.25
410	1584	1693	6.9	430	2356	2368	0.51	450	2779	2794	0.54	470	1924	1940	0.83	490	756	764	1.06
411	1610	1620	0.62	431	2398	2351	–1.96	451	2766	2834	2.46	471	1859	1882	1.24	491	714	694	–2.80
412	1637	1677	2.4	432	2440	2485	1.84	452	2750	2830	2.91	472	1795	1756	–2.18	492	674	726	7.72
413	1666	1647	–1.14	433	2480	2551	2.87	453	2729	2687	–1.54	473	1730	1714	–0.92	493	637	573	–10.05
414	1698	1725	1.59	434	2519	2505	–0.56	454	2705	2721	0.59	474	1664	1655	–0.54	494	601	576	–4.16
415	1731	1765	1.96	435	2556	2524	1.25	455	2677	2587	–3.36	475	1599	1604	0.31	495	567	553	–2.47
416	1766	1769	0.17	436	2591	2605	0.54	456	2646	2600	–1.74	476	1535	1503	–2.08	496	536	515	–3.92
417	1802	1840	2.1	437	2623	2671	1.83	457	2612	2672	2.3	477	1471	1422	–3.33	497	506	541	6.92
418	1840	1904	3.48	438	2654	2583	–2.68	458	2574	2542	–1.24	478	1407	1446	2.77	498	478	498	4.18
419	1879	1962	4.42	439	2682	2621	–2.27	459	2533	2559	1.03	479	1345	1346	0.07	499	453	432	–4.64

In Table 1, Ch: channel; Theo-val: theoretical value of spectrum after shifting; Samp-val: sampling value of spectrum after shifting; Error (%): relative error, [(Samp-val)-(Theo-val)]/(Theo-val).

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