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NOTE

Computer Simulation Study of the Properties of Orthopositronium 3γ Decay

INTRODUCTION

The three-photon annihilation of positrons and electrons is one of the fundamental quantum electrodynamics (QED) processes. Since gluons and photons are massless particles, the three-gluon decays from quarkoium are very similar to the three-photon decays from orthopositronium. Therefore the three-photon annihilation of positrons and electrons again draws the attention of many physicists.

The use of computer in the simulation test is one of the important means of comprehensively studying the properties of the three photon annihilation. The key step in the simulation test mentioned above is to realize random sampling for the three emission angles and the three energies of gamma rays.

The QED theory has predicted that when the emissive directions of the three photons are expressed as angles of α_1, α_2, α_3, as shown in Fig. 1, the probability of that the random vector $(\alpha_1, \alpha_2, \alpha_3)$ falls into the infinitesimal range nearby the given point is proportional to

$$P(\alpha_1, \alpha_2, \alpha_3) \propto [(1 - \cos\alpha_1)^2 + (1 - \cos\alpha_2)^2 + (1 - \cos\alpha_3)^2] \frac{\sin\alpha_1 \cdot \sin\alpha_2 \cdot \sin\alpha_3}{(\sin\alpha_1 + \sin\alpha_2 + \sin\alpha_3)^3}. \quad (1)$$

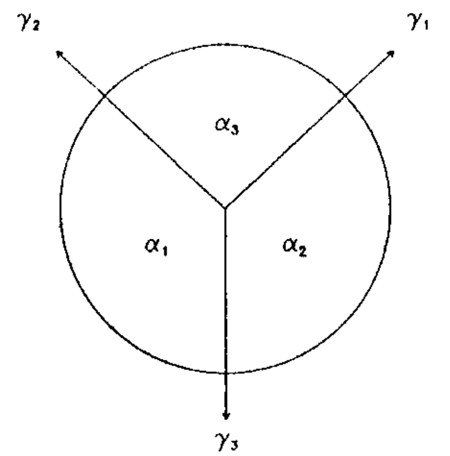

FIG. 1. Three gamma rays from positron–electron annihilation.

The definitive domain of the random vector $(\alpha_1, \alpha_2, \alpha_3)$ is $(0 < \alpha_1 < \pi, 0 < \alpha_2 < \pi, 0 < \alpha_3 < \pi, \alpha_1 + \alpha_2 + \alpha_3 = 2\pi)$. Its geometrics is the triangle-plane realm ABC, in Fig. 2. According to the law of energy-momentum conservation, the three photons are coplanar, thus the three gamma rays energy may be respectively written as

$$w_1 = g_1(\alpha_1, \alpha_2, \alpha_3) = \frac{2m_e \cdot \sin\alpha_1}{\sin\alpha_1 + \sin\alpha_2 + \sin\alpha_3} \quad (2)$$

$$w_2 = g_2(\alpha_1, \alpha_2, \alpha_3) = \frac{2m_e \cdot \sin\alpha_2}{\sin\alpha_1 + \sin\alpha_2 + \sin\alpha_3} \quad (3)$$

$$w_3 = g_3(w_1, w_2) = 2m_e - w_1 - w_2, \quad (4)$$

where $m_e = 511$ keV is the resting mass of the electron.

Generally the Metropolis method [1] is adopted for sampling the non-normalized distribution, but it is proved to be not optimum in many cases. Because $P(\alpha_1, \alpha_2, \alpha_3)$ does not satisfy the normalized condition, we use the following sampling to produce the subsamples of the matrix $(\alpha_1, \alpha_2, \alpha_3)$ and the matrix (w_1, w_2, w_3), [2] and find it works better.

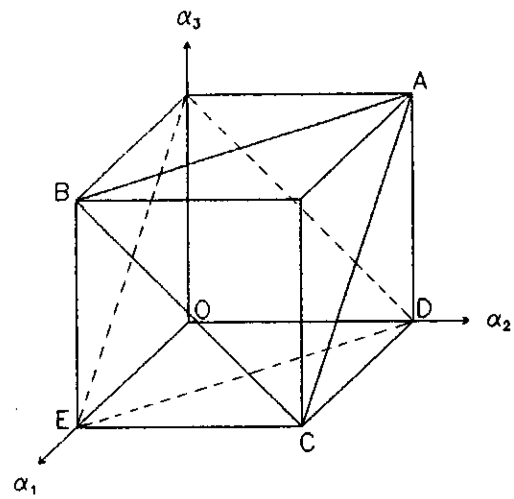

FIG. 2. The definitive domain of the random vector $(\alpha_1, \alpha_2, \alpha_3)$, i.e., the triangle-plane realm ABC.

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TECHNIQUE FOR SAMPLING

(I) Assuming that the random vector $(\alpha_1', \alpha_2', \alpha_3')$ obeys the uniform distribution in the triangle-plane realm ABC, in Fig. 2, its area is $\sqrt{3}\,\pi^2/2$. Hence we get the following probability density function

$$f(\alpha_1', \alpha_2', \alpha_3') = 2\sqrt{3}/(3\pi^2) \qquad (0 < \alpha_1' < \pi, 0 < \alpha_2' < \pi, 0 < \alpha_3' < \pi, \alpha_1' + \alpha_2' + \alpha_3' = 2\pi)$$

$$f(\alpha_1', \alpha_2') = 2/\pi^2 \qquad (0 < \alpha_1' < \pi, \pi - \alpha_1' < \alpha_2' < \pi)$$

$$f(\alpha_1') = 2\alpha_1'/\pi^2 \qquad (0 < \alpha_1' < \pi)$$

$$f(\alpha_2' | \alpha_1') = 1/\alpha_1' \qquad (\pi - \alpha_1' < \alpha_2' < \pi).$$

Therefore, we make the sampling as follows

$$\alpha_{10}' = \sqrt{\xi_1} \cdot \pi, \qquad \alpha_{20}' = \pi - \xi_2 \cdot \alpha_{10}',$$

$$\alpha_{30}' = 2\pi - \alpha_{10}' - \alpha_{20}'$$

Let $\quad E_0 = P(\alpha_{10}', \alpha_{20}', \alpha_{30}'), m = 0, n = 0.$

(II) For the determinate m, n, and E_n, we make the sampling again as follows

$$\alpha_{1(n+1)}' = \sqrt{\xi_3} \cdot \pi, \qquad \alpha_{2(n+1)}' = \pi - \xi_4 \cdot \alpha_{1(n+1)}',$$

$$\alpha_{3(n+1)}' = 2\pi - \alpha_{1(n+1)}' - \alpha_{2(n+1)}'.$$

Let $$\Delta_{n+1} = \left[(n+1)\frac{P(\alpha_{1(n+1)}', \alpha_{2(n+1)}', \alpha_{3(n+1)}')}{E_n} + \xi_5\right]$$

here $[A]$ denotes the integer part of number A.

(III) Repeat (II) if $\Delta_{n+1} < 1$, otherwise we produce the Δ_{n+1} samples of the matrix $(\alpha_1, \alpha_2, \alpha_3)$ and the matrix (w_1, w_2, w_3), respectively, as follows

$$\alpha_{1(m+1)} = \cdots = \alpha_{1(m+\Delta_{n+1})} = \alpha_{1(n+1)}'$$

$$\alpha_{2(m+1)} = \cdots = \alpha_{2(m+\Delta_{n+1})} = \alpha_{2(n+1)}'$$

$$\alpha_{3(m+1)} = \cdots = \alpha_{3(m+\Delta_{n+1})} = \alpha_{3(n+1)}'$$

$$w_{1(m+1)} = \cdots = w_{1(m+\Delta_{n+1})} = g_1(\alpha_{1(m+1)}, \alpha_{2(m+1)}, \alpha_{3(m+1)})$$

$$w_{2(m+1)} = \cdots = w_{2(m+\Delta_{n+1})} = g_2(\alpha_{1(m+1)}, \alpha_{2(m+1)}, \alpha_{3(m+1)})$$

$$w_{3(m+1)} = \cdots = w_{3(m+\Delta_{n+1})} = g_3(w_{1(m+1)}, w_{2(+1)}).$$

(IV) Let $E_{n+1} = E_n + P(\alpha_{1(n+1)}', \alpha_{2(n+1)}', \alpha_{3(n+1)}')$, $m = m + \Delta_{n+1}$, $n = n + 1$. Repeat the steps (II)–(IV) until $m \geq N$.

In the above expressions the ξ_1, ξ_2, ξ_3, ξ_4, and ξ_5 are the random numbers uniformly distributed in the region (0, 1).

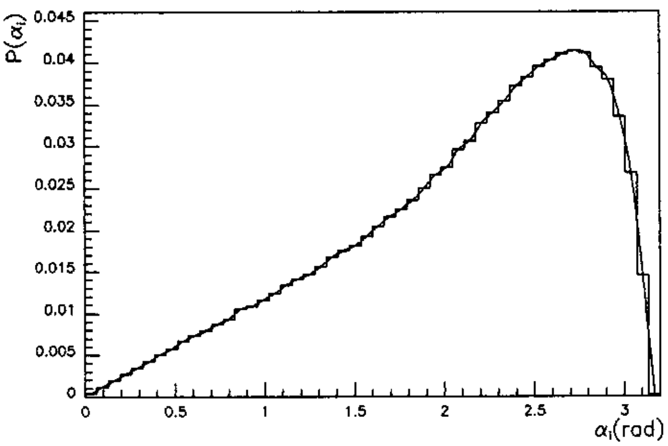

FIG. 3. The angular distribution of gamma rays emitted in the three-photon annihilation of positrons and electrons (marginal distribution).

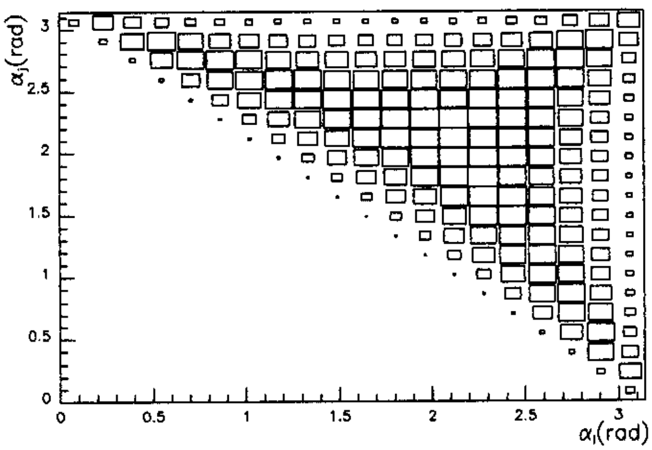

FIG. 4. The probability distribution of the random vector $(\alpha_1, \alpha_2, \alpha_3)$.

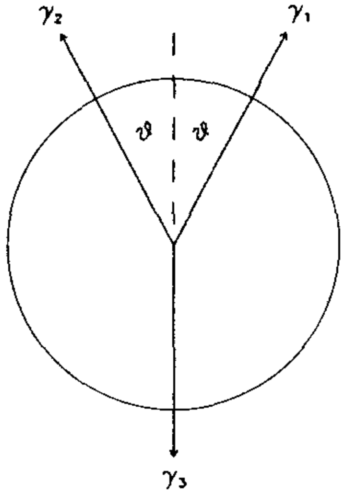

FIG. 5. Three gamma rays from incompletely symmetric positron–electron annihilation.

CONCLUSIONS

According to the subsamples generated by the sampling mentioned above, we have drawn the following conclusions.

(I) The random variables $\alpha_1, \alpha_2, \alpha_3$ have an identical front-dominated distribution. It is a continuous distribution in the angle range from 0 to π, as shown in Fig. 3.

(II) The numeral values in Fig. 4 indicate the probability which is projected on the plane $o - \alpha_i\alpha_j$ $(i, j = 1, 2, 3; i \neq j)$ when the random vector $(\alpha_1, \alpha_2, \alpha_3)$ falls into the given region on its definitive domain. From Figs. 4 and 2, we have found that the probability distribution of the random vector $(\alpha_1, \alpha_2, \alpha_3)$ has a symmetry in its definitive domain. The axis of symmetry is any one of the midlines of the triangle ABC shown in Fig. 2.

(III) When the three-photon emission is incompletely symmetric, as shown in Fig. 5, our computational results are in good agreement with the experimental data in Ref. [3] (see Fig. 6).

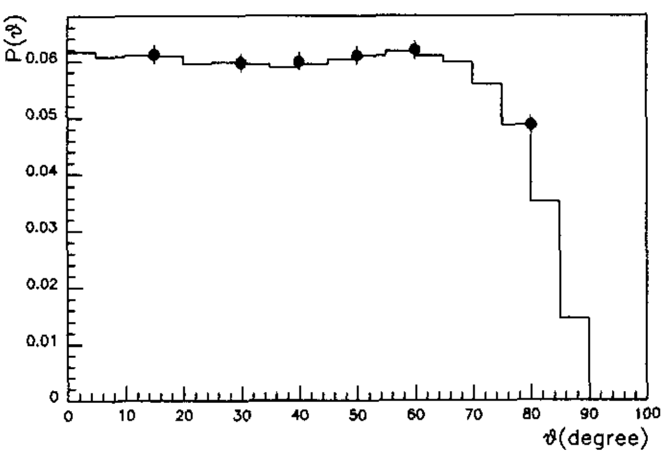

FIG. 6. The angular distribution of gamma rays emitted in the incompletely symmetric three photon annihilation. The histogram is our computational result. The points are the experimental data of Ref. (3).

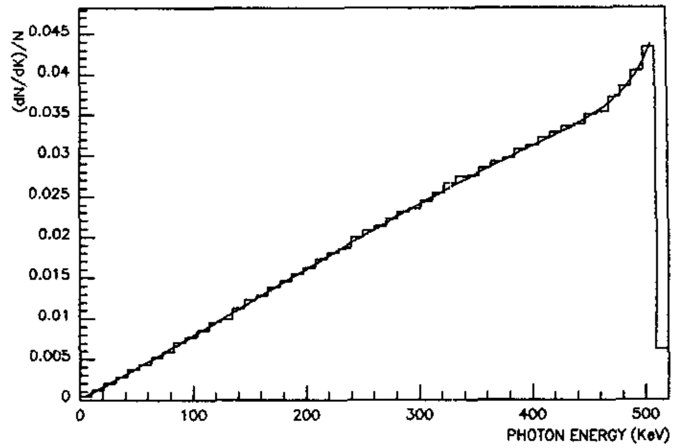

FIG. 7. The normalized energy spectrum of the gamma ray emitted in the three-photon annihilation of positrons and electrons.

(IV) The random variables w_1, w_2, w_3 have an identical front-dominated distribution, too. It is a continuously rising distribution in the energy range from 0 to 511 keV, as shown in Fig. 7. The experimental and theoretical energy spectra of the gamma rays emitted in the three-photon annihilation of positrons and electrons are shown in Fig. 8. Because the QED theory curve in Fig. 8 is the graph of function $g(k)$

$$g(k) = \frac{1}{3}\left[\frac{k(m_e - k)}{(2m_e - k)^2} - \frac{2m_e(m_e - k)^2}{(2m_e - k)^3}\ln\frac{m_e - k}{m_e} + \frac{2m_e - k}{k} + \frac{2m_e(m_e - k)}{k^2}\ln\frac{m_e - k}{m_e}\right] \tag{5}$$

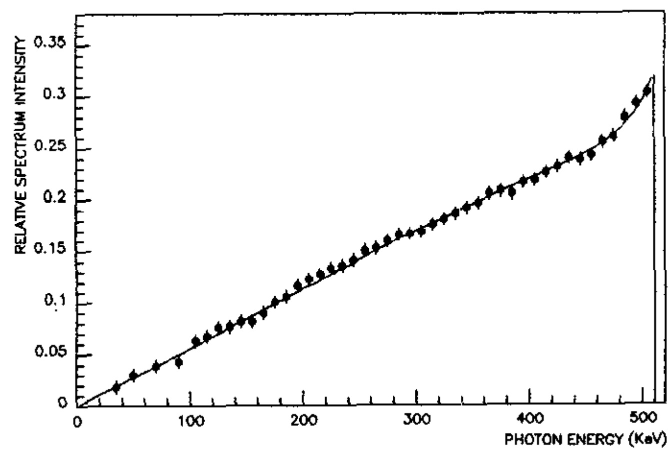

FIG. 8. The experimental and theoretical energy spectra of the gamma ray emitted in the three photon annihilation of positrons and electrons. The solid curve is the QED theoretical energy spectrum of Ref. (5). The points are the experimental data of Ref. (6).

TABLE I

Some Values of $g(k)$ and $f(k)$

$g(k)$	0.002	0.004	0.007	0.010	0.012	0.015	0.018	0.021	0.023	0.026	0.029	0.032	0.035	0.038	0.040	0.043	0.046
$f(k)$	0.001	0.004	0.006	0.010	0.011	0.016	0.018	0.020	0.023	0.029	0.028	0.031	0.034	0.037	0.040	0.044	0.045
$g(k)$	0.049	0.052	0.055	0.058	0.061	0.064	0.066	0.069	0.072	0.075	0.078	0.081	0.084	0.087	0.090	0.093	0.096
$f(k)$	0.050	0.052	0.056	0.060	0.060	0.062	0.067	0.070	0.070	0.076	0.081	0.083	0.086	0.087	0.089	0.093	0.095
$g(k)$	0.099	0.102	0.105	0.108	0.110	0.113	0.116	0.119	0.122	0.125	0.128	0.131	0.134	0.137	0.140	0.142	0.145
$f(k)$	0.100	0.101	0.105	0.110	0.110	0.115	0.115	0.119	0.122	0.125	0.127	0.131	0.133	0.139	0.138	0.140	0.146
$g(k)$	0.148	0.151	0.154	0.157	0.159	0.162	0.165	0.168	0.171	0.173	0.176	0.179	0.181	0.184	0.187	0.189	0.192
$f(k)$	0.149	0.152	0.155	0.156	0.157	0.159	0.163	0.168	0.169	0.172	0.179	0.180	0.184	0.184	0.186	0.188	0.192
$g(k)$	0.194	0.197	0.199	0.202	0.204	0.207	0.209	0.212	0.214	0.216	0.219	0.221	0.224	0.226	0.228	0.231	0.233
$f(k)$	0.196	0.197	0.199	0.201	0.204	0.208	0.211	0.212	0.215	0.215	0.220	0.221	0.224	0.225	0.228	0.231	0.230
$g(k)$	0.236	0.238	0.241	0.244	0.246	0.249	0.253	0.256	0.260	0.264	0.268	0.273	0.279	0.286	0.294	0.304	0.319
$f(k)$	0.234	0.238	0.239	0.246	0.243	0.248	0.251	0.256	0.260	0.266	0.271	0.276	0.278	0.284	0.294	0.305	0.319

and from Ref. 4 we get

$$C = \int_o^{m_e} g(k)\, dk = \frac{m_e}{6}(\pi^2 - 9).$$

Therefore we expand C times of our computational results and have

$$f(k) = C \cdot \frac{1}{N}\frac{dN}{dk}, \tag{6}$$

where k is the gamma ray energy.

Some values of $g(k)$ and $f(k)$ are shown in Table I. From Table I we get

$$\max_{1 \le i \le 102} |g(k_i) - f(k_i)| = 0.003,$$

where $k_i = 5i - 2.5$ keV ($i = 1, 2, ..., 101$) and $k_{102} = 508$ keV.

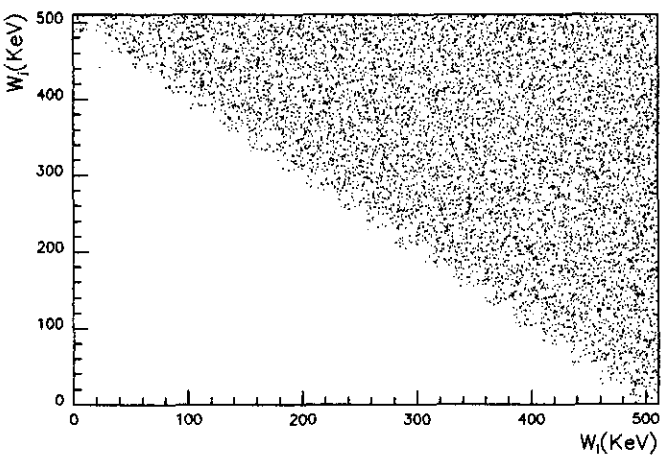

FIG. 9. The probability distribution of the random vector (w_1, w_2, w_3).

We also performed the χ^2 test for our computational results and obtained

$$\chi^2(101) = \sum_{j=1}^{102} [(n_j - N \cdot p_j)^2/(N \cdot p_j)] = 30.2,$$

where

$$p_j \approx g[(k_j + k_{j-1})/2](k_j - k_{j-1})/C$$

$$k_j = 5j \text{ keV} \qquad (j = 1, 2, ..., 101)$$

$$k_o = 0, \qquad k_{102} = 511 \text{ keV}$$

and n_j is the practical frequency.

The computational results mentioned above show that when the identical unit is adopted for these three spectra, in Figs. 7 and 8, they are in accord quite well. We have also obtained that the random vector (w_1, w_2, w_3) approximately obeys the uniform distribution in its definitive domain, as shown in Fig. 9, which is ($0 < w_1 < 511$ keV, $0 < w_2 < 511$ keV, $0 < w_3 < 511$ keV, $w_1 + w_2 + w_3 = 1022$ keV).

(V) The results of the analysis mentioned above show that the subsamples, which are produced by the sampling presented in this paper, reflect the circumstances of the matrixes quite well. This sampling is very efficient.

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