A Fundamental Limit on Timing Performance with Scintillation Detectors

Neal H. Clinthorne, Nick A. Petrick, W. Leslie Rogers, and Alfred O. Hero III
The University of Michigan, Division of Nuclear Medicine and
Dept. of Electrical Engineering and Computer Science.
Ann Arbor, MI 48109-0552.

Abstract

A new lower bound on the mean-squared error of post-detection γ-ray time-of-flight estimators has been derived. Previously, the Cramer-Rao bound has been applied, but for nearly exponentially decaying scintillation pulses it gives an extremely optimistic picture of the achievable performance, depending critically on the dark current and photomultiplier characteristics.

The new bound has been derived under the assumption that excited states in the scintillator leading to the emission of scintillation photons have an exponential lifetime density. The bound is a function of the mean state lifetime, the spectrum of energy deposited, and the energy conversion efficiency of the scintillator, and is exact for the observation of a mono-exponentially decaying photoelectron rate at the first dynode of the PMT given the γ-ray arrival time.

I. INTRODUCTION

Recent investigations have focused on improving the timing performance of scintillation detectors with the goals of both improving the resolution of PET time-of-flight scanners and reducing the accidental coincidence rate in conventional PET tomographs. Tomitani investigated the performance of maximum-likelihood time-of-flight estimates, assuming that the point-process of photoelectron arrivals at the first dynode could be directly observed [1]. More recently, Hero, et al. have expanded a model used in optical communications, which includes PMT statistics and have derived approximately optimal time-of-flight estimators [2].

A possible disadvantage of these more optimal timing estimators is that they may greatly increase the processing requirements for each scintillation while only resulting in marginal performance gains over present methods. Lower bounds on the ultimate timing performance can be useful in assessing the degree of suboptimality of present timing techniques and in identifying regimes where a considerable gain may be realized using an optimized method. The Cramer-Rao (CR) bound has been employed to assess timing performance, but in situations where the scintillation pulse is rapidly varying, such as a mono-exponential pulse, the CR bound tends to exaggerate the achievable performance by stating that the mean-squared error must be greater than or equal to zero.

Recognizing this deficiency of the CR bound, we derive a lower bound on the post-detection mean-squared timing error, assuming that the prior uncertainty in γ-ray arrival time is much greater than the post-detection uncertainty. Since PMT statistics are difficult to meaningfully describe thoeretically, the bound assumes direct observation of the point-process of photoelectrons at the first dynode and uses the model that the excited states in the scintillator leading to luminescence have an exponential lifetime density. The bound is the exact mean-squared error for a mono-exponentially decaying scintillation with no dark current.

II. SCINTILLATOR / PMT MODEL

Timing degradations in scintillation detectors arise from many sources including (1) the time required for a γ-ray to transfer its energy to the scintillator lattice and populate excited states, (2) the random lifetime of these excited states leading to release of scintillation photons, (3) the optical collection statistics of scintillation photons at the photocathode, (4) conversion of photons to photoelectrons, (5) transit time jitter preceding collection at the first dynode, and (6) PMT multiplication statistics. In the subsequent development, we assume that the photoelectron arrival times at the first dynode can be directly observed and that their statistics can be represented by a Poisson point-process model [3]. It is instructive at this point to review the assumptions inherent in this model.

When a γ-ray crosses the fiducial or timing plane of a scintillator, its energy is instantaneously converted into a number of equivalent quanta which are Poisson distributed with mean $\Lambda_0(h\nu)$, where $h\nu$ is the energy *deposited* by the γ-ray. These hypothetical quanta then travel through a cascade of degradation processes independently and at each stage experience the same random effects in which (1) a quantum may be absorbed with probability $(1-\eta_i)$ or (2) the quantum may be successfully transferred to the next stage with probability η_i after being held for a random

This work was supported by the National Cancer Institute, DHHS, under PHS grant CA46622.

0018-9499/90/0400-0658$01.00 © 1990 IEEE

time in accordance with the probability density function (pdf) $f_i(t_i|t_{i-1})$. Accounting for n stages of degradations, the mean rate of photoelectron arrivals at the first dynode given the γ-ray arrival time τ and deposited energy is given by the $(n-1)$-fold convolution,

$$\lambda_S(t-\tau) = \Lambda_0(h\nu)\eta_1\cdots\eta_n \times \tag{1}$$
$$\int_0^\infty \cdots \int_0^\infty f_n(t-\sigma_{n-1})\cdots f_1(\sigma_1-\tau)d\sigma_1\cdots d\sigma_{n-1},$$

where the overall conversion of energy to mean number of photoelectrons is given by $\Lambda = \Lambda_0(h\nu)\eta_1\cdots\eta_n$ and the timing effects are described by the convolution of the pdfs, $f_i(t_i-t_{i-1})$, which are assumed to be causal and time-invariant. This model describes all degradation effects except the photomultiplication statistics. Note that if this model truly applied, the number of photoelectrons observed due to a scintillation would be a Poisson random variable with mean Λ, conditioned on the deposited energy. Although there is a good deal of evidence suggesting that this is not the case [4], the expressions developed in Section IV can still be applied as lower bounds.

Inspection of (1) reveals that since the timing degradation pdfs are time-invariant, we can represent the intensity in a more convenient fashion by rearranging orders of integration and making appropriate changes in variables. The following representation will be used in the sequel although others are certainly possible.

$$\lambda_S(t-\tau) = \int_0^\infty g(\sigma)\lambda(t-\sigma-\tau). \tag{2}$$

Here the intensity $\lambda(t-\tau)$ is the product of Λ and the pdf describing the lifetime of the excited states whose decay leads to the production of scintillation photons and $g(\sigma)$ is a pdf combining the effects of all other degradations. Note that (2) represents an *energy-constrained* smoothing of the intensity $\lambda(t-\tau)$.

In addition to the photoelectron arrivals due to a scintillation, there is often a background process of photoelectrons arriving independently of the current scintillation. This possibly time-varying background is added to (2) to obtain the observed rate of photoelectron arrivals at the first dynode,

$$\lambda_C(t,\tau) = \lambda_S(t-\tau) + \lambda_D(t), \tag{3}$$

where $\lambda_D(t)$ is the mean background rate.

The conditional pdf or *likelihood* of observing a given sequence of arrival times, $\{t_i\}_{i=1}^{N_T}$, and number of photoelectrons, N_T, on the interval [0,T] is given by

$$f(\{t_i\}_{i=1}^{N_T}, N_T|\tau) = e^{-\Lambda_C(T,\tau)}\prod_{i=1}^{N_T}\lambda_C(t_i,\tau), \tag{4}$$

where $\Lambda_C(T,\tau)$ is (3) integrated over the interval $[0,T]$.

III. MINIMUM MEAN-SQUARED ERROR ESTIMATION

The MSE, defined as the average loss or error associated with the estimator $\hat{\tau} = \hat{\tau}(\{t_i\}_{i=1}^{N_T}, N_T)$ and the pdf defined in (4), can be written as:

$$E((\tau-\hat{\tau})^2) = \sum_{N_T=0}^{\infty}\frac{1}{N_T!}\times \tag{5}$$
$$\int_0^T dt_1\cdots\int_0^T dt_{N_T}\int_0^T(\tau-\hat{\tau})^2 f(\{t_i\}_{i=1}^{N_T}, N_T|\tau)f(\tau)d\tau,$$

where τ is the true arrival time, $f(\tau)$ is the prior pdf of this arrival time and the scintillation is observed on the interval $[0,T]$.

The minimum mean-squared error (MMSE) estimator of the arrival time, τ, is the conditional mean of τ given the direct observation of the point-process of photoelectron arrivals at the first dynode

$$\begin{aligned}\hat{\tau}_{mmse} &= E[\tau|\{t_i\}_{i=1}^{N_T}, N_T] \\ &= \frac{\int_0^T \tau e^{-\Lambda_C(t,\tau)}\prod_{i=1}^{N_T}\lambda_C(t_i,\tau)f(\tau)d\tau}{\int_0^T e^{-\Lambda_C(t,\tau)}\prod_{i=1}^{N_T}\lambda_C(t_i,\tau)f(\tau)d\tau}.\end{aligned} \tag{6}$$

In principle, the best-case MSE performance can be calculated by evaluating (6) using the optimal estimate defined by (7). Unfortunately, for all but the simplest intensity functions, this can be exceedingly difficult—even numerically. To develop a lower bound on the MSE we first state two rather intuitive propositions omitting proofs which follow directly from the above definitions.

Propostion 1:
The mean-squared error using the intensity, $\lambda_C(t,\tau)$ defined above, is lower bounded by the minimum mean-squared error attainable with the intensity having no dark current, $\lambda_S(t-\tau)$.

Proposition 2:
The mean-squared timing error using the energy-constrained, smoothed intensity $\lambda_S(t-\tau)$ is lower bounded by the minimum mean-squared error with the unsmoothed intensity $\lambda(t-\tau)$.

In the next section, we combine these results with the decompostion of the intensity allowed by (2) to derive an easy to evaluate lower bound on the mean-squared timing error for any scintillator having excited states leading to luminescence which have an exponential lifetime density.

IV. LOWER BOUND ON TIMING MSE

Single state lifetime
A common model for the unsmoothed scintillation intensity is the monoexponentially decaying pulse,

$$\lambda(t-\tau) = \begin{cases} \Lambda\tau_1^{-1}e^{-(t-\tau)/\tau_1} & \text{if } t \geq \tau \\ 0 & \text{otherwise.}\end{cases}$$

where τ_1 is the mean state lifetime or *decay constant.*

Assuming that $f(\tau)$, the prior pdf of the γ-ray arrival time, is uniform over an interval, $[0, T]$, much longer than the mean lifetime, τ_1, the MMSE estimator takes the form,

$$\tau_{mmse} = \min\{t_i\}_{i=1}^{N_T} - \frac{\tau_1}{N_T}, \quad (7)$$

or the arrival time of the first electron corrected for a bias depending on the mean lifetime and observed number of photoelectrons, N_T. This result was first derived by Bar-David [5].

The MSE performance of this estimator can be calculated using the first photoelectron arrival pdf,

$$f(t_{min}|N_T, \tau) = \frac{N_T}{\tau_1} e^{-N_T(t-\tau)/\tau_1}, \quad t \geq \tau. \quad (8)$$

and since the post-detection timing performance is desired, we condition on the event that we have collected at least one photoelectron. The resulting MSE, also conditioned on the γ-ray energy, $h\nu$, is

$$\begin{aligned} \overline{D^2} &\geq E[(\tau - \hat{\tau}_{mmse})^2 | N_T \geq 1, h\nu] \\ &= \tau_1^2 E(N_T^{-2} | N_T \geq 1, h\nu), \end{aligned} \quad (9)$$

where $\overline{D^2}$ represents the MSE with the actual intensity, $\lambda_C(t)$, and the expectation on the second line is taken over the Poisson distribution having mean, $\Lambda(h\nu) = \Lambda_0(h\nu)\eta_1 \cdots \eta_n$, defined in Section II. If there is a broad spectrum of incident energies, (9) can also be averaged over this spectrum to obtain a lower bound on the unconditional MSE.

It is interesting to note that for moderate mean photoelectron numbers ($\Lambda(h\nu) > 120$), this expression is within 1% of the approximation developed by Post and Schiff based on the mean rate of first photoelectron arrivals [6].

$$\overline{D^2} \geq E[(\tau - \hat{\tau}_{mmse})^2 | N_T \geq 1, h\nu] \approx \frac{\tau_1^2}{\Lambda(h\nu)^2}. \quad (10)$$

Extension to Multiple Lifetimes

The expression developed above assumes that all photoelectrons reaching the first dynode are sequestered in excited states having a single mean lifetime. Commonly, the scintillator output is more accurately described by a mixture of exponentially decaying pulses due to excited states having multiple decay constants.

For a scintillator with two characteristic decay constants, τ_1 and τ_2, we can write the unsmoothed intensity as,

$$\lambda(t-\tau) = \begin{cases} \Lambda \left[\frac{\alpha}{\tau_1} e^{-(t-\tau)/\tau_1} + \frac{(1-\alpha)}{\tau_2} e^{-(t-\tau)/\tau_2}\right] & t \geq \tau \\ 0 & t < \tau, \end{cases}$$

where α describes the average relative mixture of states and $0 \leq \alpha \leq 1$.

Solving directly for the MMSE estimator for the above intensity is difficult. However, suppose that for each scintillation, we can additionally observe the number of states populated having each mean lifetime. Representing the number of excited states with lifetime τ_1 by L_T and with lifetime τ_2 by M_T, we can write the likelihood function as the sum of $(L_T + M_T)!$ terms of the form,

$$f(\{t_i\}_{i=1}^{L_T+M_T} | L_T, M_T, O_k, \tau) = \quad (11)$$
$$\tau_1^{-L_T} \tau_2^{-M_T} \prod_{i=1}^{L_T} e^{-(t_i^{S1}-\tau)/\tau_1} \prod_{j=1}^{M_T} e^{-(t_j^{S2}-\tau)/\tau_2},$$

where O_k represents one of the $(L_T + M_T)!$ permutations of the arrival times among the states and where $\{t_i^{S1}\}_{i=1}^{L_T}$ and $\{t_j^{S2}\}_{j=1}^{M_T}$ are the sequences of arrival times assigned to states with decay constants τ_1 and τ_2 respectively.

Substituting this new likelihood into (7) and taking the prior density, $f(\tau)$, to be uniform as above, results in the desired MMSE estimator,

$$\hat{\tau}_{mmse} = \min\{t_i\}_{i=1}^{L_T+M_T} - \left[\frac{L_T}{\tau_1} + \frac{M_T}{\tau_2}\right]^{-1}. \quad (12)$$

Calculating the MSE conditioned on M_T and L_T using the the first photoelectron pdf,

$$f(t_{min}|L_T, M_T, \tau) = \quad (13)$$
$$\left[\frac{L_T}{\tau_1} + \frac{M_T}{\tau_2}\right] \exp\left[-\left(\frac{L_T}{\tau_1} + \frac{M_T}{\tau_2}\right)(t-\tau)\right], \quad t \geq \tau$$

results in the expression,

$$E[(\tau - \hat{\tau}_{mmse})^2 | L_T, M_T, h\nu] = \left[\frac{L_T}{\tau_1} + \frac{M_T}{\tau_2}\right]^{-2}. \quad (14)$$

Averaging over the Poisson distributed random variables L_T and M_T having means $\alpha\Lambda(h\nu)$ and $(1-\alpha)\Lambda(h\nu)$, and conditioning on the event that $L_T + M_T \geq 1$ yields the desired lower bound. Again, for moderate values of $\Lambda(h\nu)$, the following approximation is quite reasonable

$$\begin{aligned} \overline{D^2} &\geq E[(\tau - \hat{\tau}_{mmse})^2 | L_T + M_T \geq 1, h\nu] \\ &\approx \Lambda^{-2}(h\nu) \left[\frac{\alpha}{\tau_1} + \frac{(1-\alpha)}{\tau_2}\right]^{-2}. \end{aligned} \quad (15)$$

Cramer-Rao Lower Bound

The global Cramer-Rao (CR) bound on the MSE was introduced by VanTrees and for the likelihood function (4) and prior pdf of γ-ray arrival time, $f(\tau)$, takes the form,

$$\overline{D^2} \geq \left[\int_0^T \frac{(\partial\lambda(\tau)/\partial\tau)^2}{\lambda(\tau) + \lambda_D} d\tau + E\left(\frac{\partial \ln f(\tau)}{\partial\tau}\right)^2\right]^{-1}, \quad (16)$$

where λ_D is assumed to be a constant dark current [7]. We see that this bound requires that both the intensity and prior density be differentiable. However even if these conditions are satisfied, the bound tends to be overly optimistic for any intensity which changes abruptly where $\lambda(t) + \lambda_D$ is small.

V. COMPARISONS WITH MONTE-CARLO

We compared the bounds of Section IV with bias-corrected "first-photoelectron" timing (FPET) results obtained from Monte-Carlo simulations incorporating a PMT model. We chose an unsmoothed intensity function having two exponenetially decaying components with parameters typical of BGO ($\tau_1 = 60ns$, $\tau_2 = 300ns$, $\alpha = 0.1$, [8]). To assess the effects of additional timing degradations and to allow evaluation of the CR bound, we also performed simulations using the above intensity smoothed with a $2ns$ fwhm gaussian.

The output current of the PMT was modeled by the superposition of "impulse responses" having constant shape, $p(t)$, but randomly scaled by the gain for each photoelectron, β_j. The expression relating the output current, $i(t)$, to the point-process of photoelectrons, $\{t_j\}_{j=1}^{N_T}$, is

$$i(t) = \sum_{j=1}^{N_T} \beta_j p(t - t_j) + \mathrm{w}(t), \qquad (17)$$

where $\mathrm{w}(t)$ is an additive white noise term modeling the thermal electronic noise. We assume that the random gains β_j are independent, identically distributed (i.i.d.), and drawn from a known pdf. This model, excluding the white noise term, has been successfully applied to modeling the observed pulse-height distribution from phototubes [9].

To use realistic parameters in (17), the single-photoelectron gain distribution was measured for a Burle/RCA 8850 PMT using the technique described in [10] and is shown in figure 1. The impulse response shape for this PMT was measured using full photocathode illumination with an Antel Optronics PL-670 diode laser pulser (67ps fwhm, 670nm) and the output current was sampled with a Stanford Research Systems SR255 sampler using a 100 ps gate width. The measured impulse response is shown in figure 2. Since full photocathode illumination was employed we expect that this is somewhat broader than the true time response to a single-photoelectron.

First photoelectron timing was simulated by generating a γ-ray arrival time from the prior density, $f(\tau)$, and then the point-process of photoelectron arrivals initiated by the γ-ray. Random gains were were drawn from the pdf in figure 1 and (17) was applied to simulate the phototube output current. The simulated current was applied to a threshold detector and the first threshold-crossing in the interval $[0, T]$ was taken as the arrival time estimate. Two photoelectron detection thresholds were used and are illustrated in figure 1. To create an ideal situation for FPET, the white noise term in (17) was set to zero and there was no dark current.

The results for the unsmoothed intensity are presented in figure 3 where the RMS timing error in nanoseconds is plotted against the base 10 log of the mean number of photons in a scintillation.. The prior density of γ-ray arrival time was chosen to be gaussian with a variance much

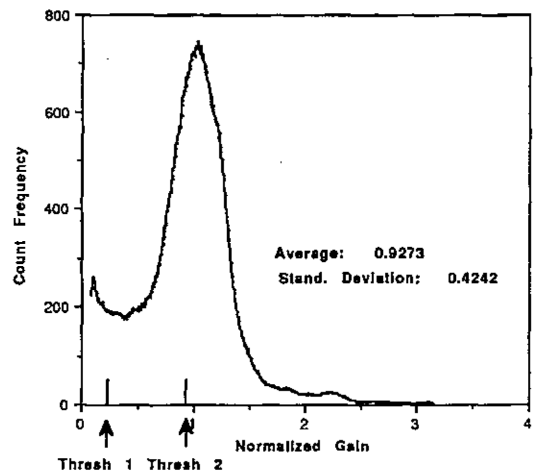

Figure 1: Single photoelectron gain distribution for Burle/RCA 8850 PMT. The two FPET discriminator thresholds are also shown.

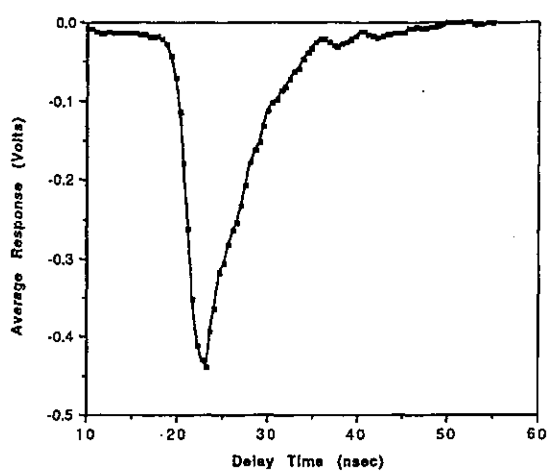

Figure 2: Impulse response for Burle/RCA 8850 PMT measured with full photocathode illumination.

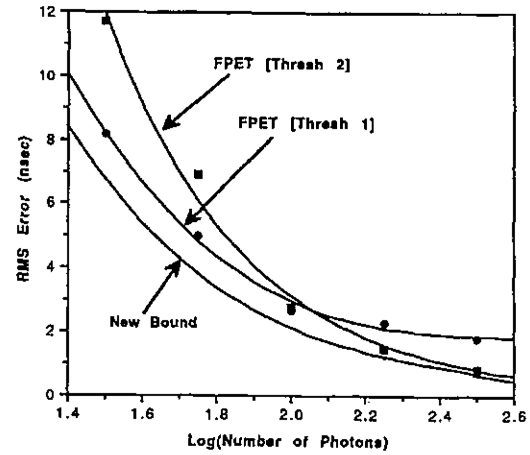

Figure 3: Results of Monte-Carlo FPET simulations plotted against lower bound for unsmoothed intensity

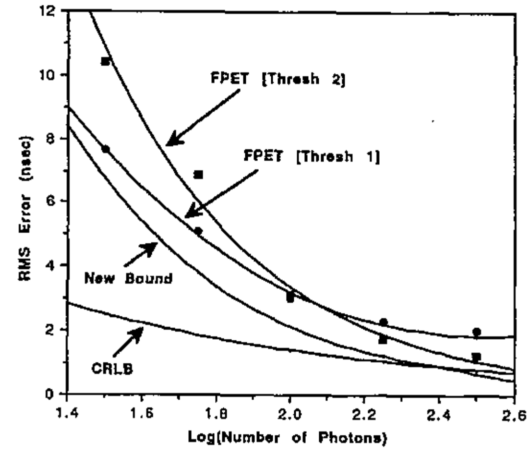

Figure 4: Results of FPET simulations using intensity smoothed by 2 ns fwhm gaussian. The CR bound is plotted along with the new bound.

larger than τ_2 so that the MMSE estimator (12) was optimal. The CR bound cannot be evaluated for this intensity and is not shown. The new lower bound is plotted along with the results of the Monte-Carlo FPET simulations using two discriminator settings for detection. Note that the FPET performance with increasing Λ follows the bound very well for the lower discriminator setting at low photoelectron rates. At higher rates, the broader range of pulse heights resulting from this threshold actually degrades performance and the higher detection threshold approaches the limiting time resolution. For the FPET method to perform as well as this predicts requires that the additive white noise and dark current be nearly absent.

The situation for the same intensity smoothed by a 2 ns fwhm gaussian is shown in figure 4. Here the CR bound can be evaluated and is plotted along with the new bound and FPET simulations with the same discriminator settings as above. At low photoelectron levels the new bound is a better performance indicator than the CR bound, but at higher levels the CR bound eventually dominates because its rate of improvement is only $O(\Lambda^{1/2})$. In this low background noise situation, FPET still performs remarkably well relative to the limits.

VI. CONCLUSION

A new lower bound on the achievable mean-squared timing error has been presented. The bound overcomes the deficiencies of the Cramer-Rao bound for both low photoelectron rates and exponentially decaying scintillation pulses. However, in cases where additional smoothing may be present in the scintillation, the Cramer-Rao bound eventually dominates as the photoelectron rate is increased. This additional smoothing may arise from PMT transit-time jitter or optical collection time dispersion in long scintillators. However, results from simulations of first photoelectron timing, using a PMT and scintillator model suggest that these fundamental limits can be nearly achieved with present timing methods at moderate mean photoelectron rates such as those that might be observed with BGO at 511 keV.

References

[1] Tomitani T, "A Maximum Likelihood Approach to Timing in Scintillation Counters," *Proceedings of the IEEE Workshop on Time-of-Flight Tomography,* Vol. 1, pp. 88–93, May 1982.

[2] Hero AO, Antoniadis N, Clinthorne NH, Rogers WL, Hutchins GD, "Optimal Post-Detection Timing Estimators for PET," *Presented at the 1989 IEEE Nuclear Science Symposium,* San Francisco, CA, January 1990.

[3] Snyder DL, *Random Point Processes,* Wiley, New York, NY 1975.

[4] Narayan GH, Prescott JR, "The Contribution of the NaI(Tl) Crystal to the Total Linewidth of NaI(Tl) Scintillation Counters." *IEEE Trans. on Nucl. Sci.,* NS-15(3):162–166, 1968.

[5] Bar-David I, "Minimum Mean-Square-Error Estimation of Photon Pulse Delay," *IEEE Trans. on Inform. Theory*, 326–330, May 1975.

[6] Post RF, Schiff LI, Statistical limitations on the resolving time of a scintillation counter. *Phys. Rev.*, 80:1113, 1950.

[7] VanTress HL, *Detection, Estimation, and Modulation Theory: Vol I*, Wiley, New York, NY, 1969.

[8] Moszynski M, Gresset C, Vacher J, Odru R, "Timing Properties of BGO Scintillator," *Nuclear Instruments and Methods* 188:403–409, 1981.

[9] Wright AL, "A Monte Carlo Simulation of Photomultiplier Resolution," *IEEE Trans. Nucl. Sci.*, NS-34:414–417, Feb. 1987.

[10] *RCA Photomultiplier Handbook*, pp. 59–60, RCA, Lancaster, PA, 1980.