Optimal Detection of Single Spin MR

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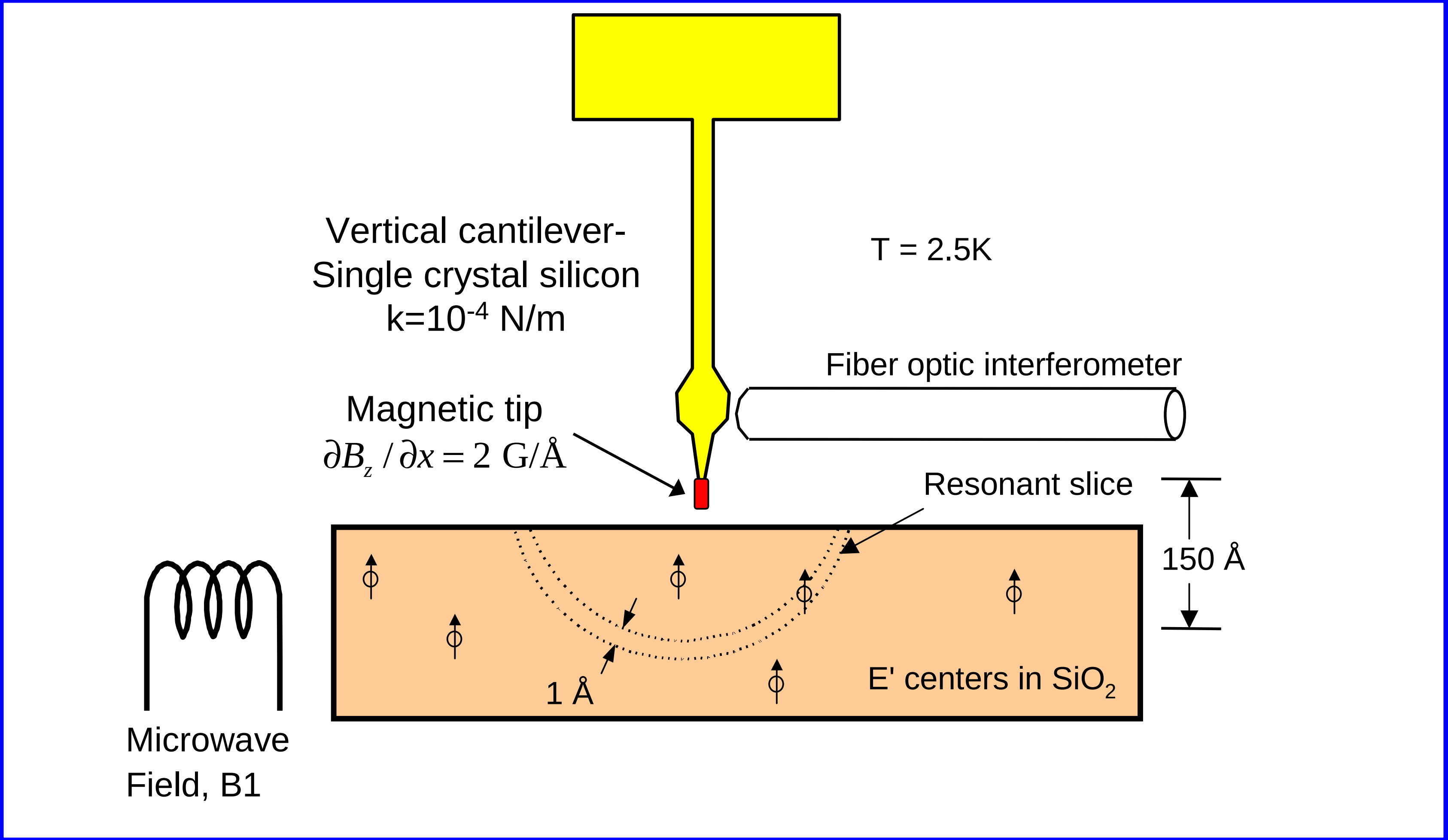
Outline

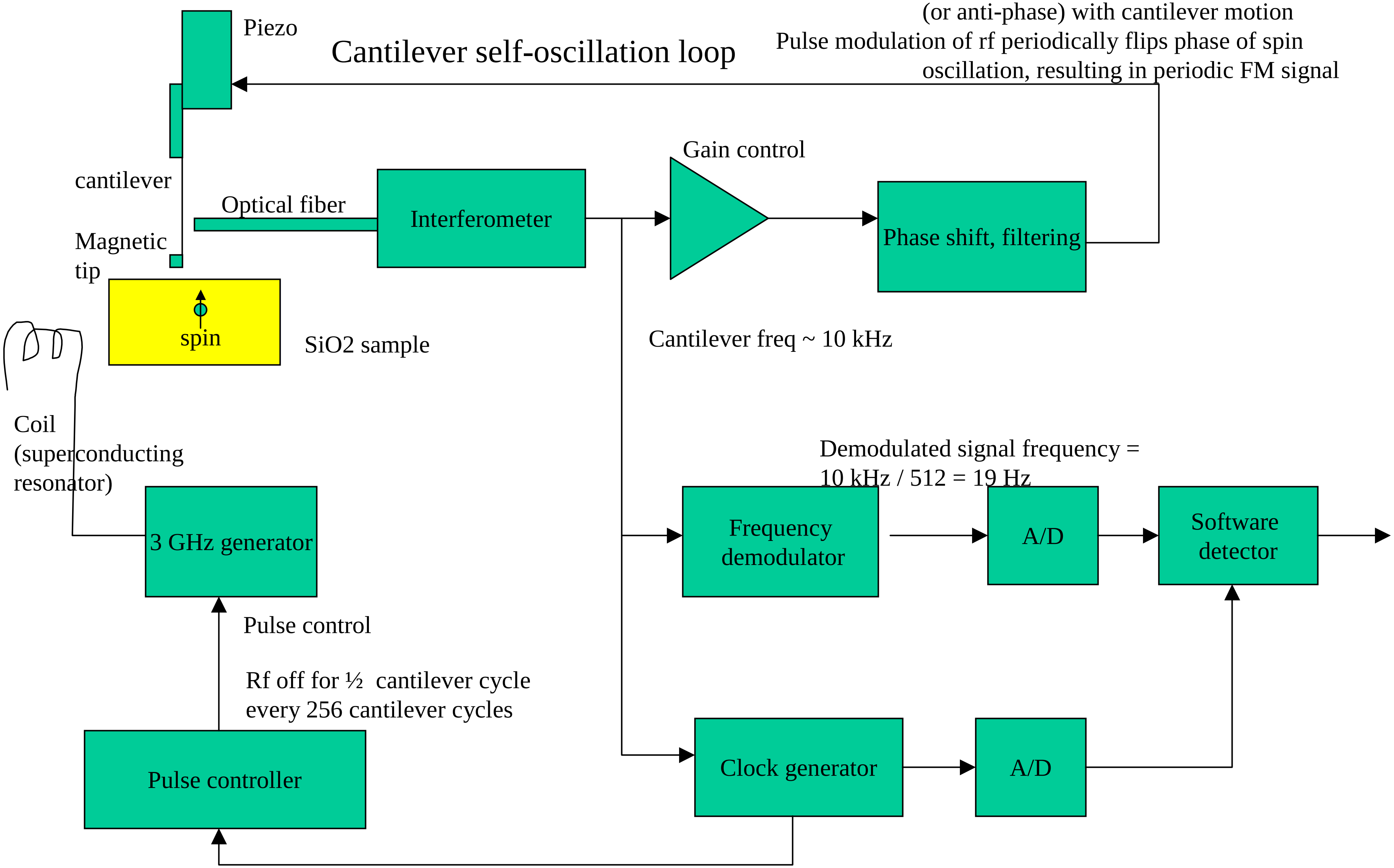
- Cantilever-based single spin measurement system
- Signal detection framework
- Areas of research

Single Electron Spin MRFM Experiment



- Vibrate tip and induce cyclic adiabatic inversion using 6 GHz microwave field
- Resulting force signal is 13 aN-rms
- Signal is measured via cantilever frequency shift

Cantilever oscillates at natural frequency with ~20 nm amplitude
Cantilever motion induces synchronous spin flips when rf is on
Cantilever frequency shifted up (or down) when spin flip in phase (or anti-phase) with cantilever motion
Pulse modulation of rf periodically flips phase of spin oscillation, resulting in periodic FM signal



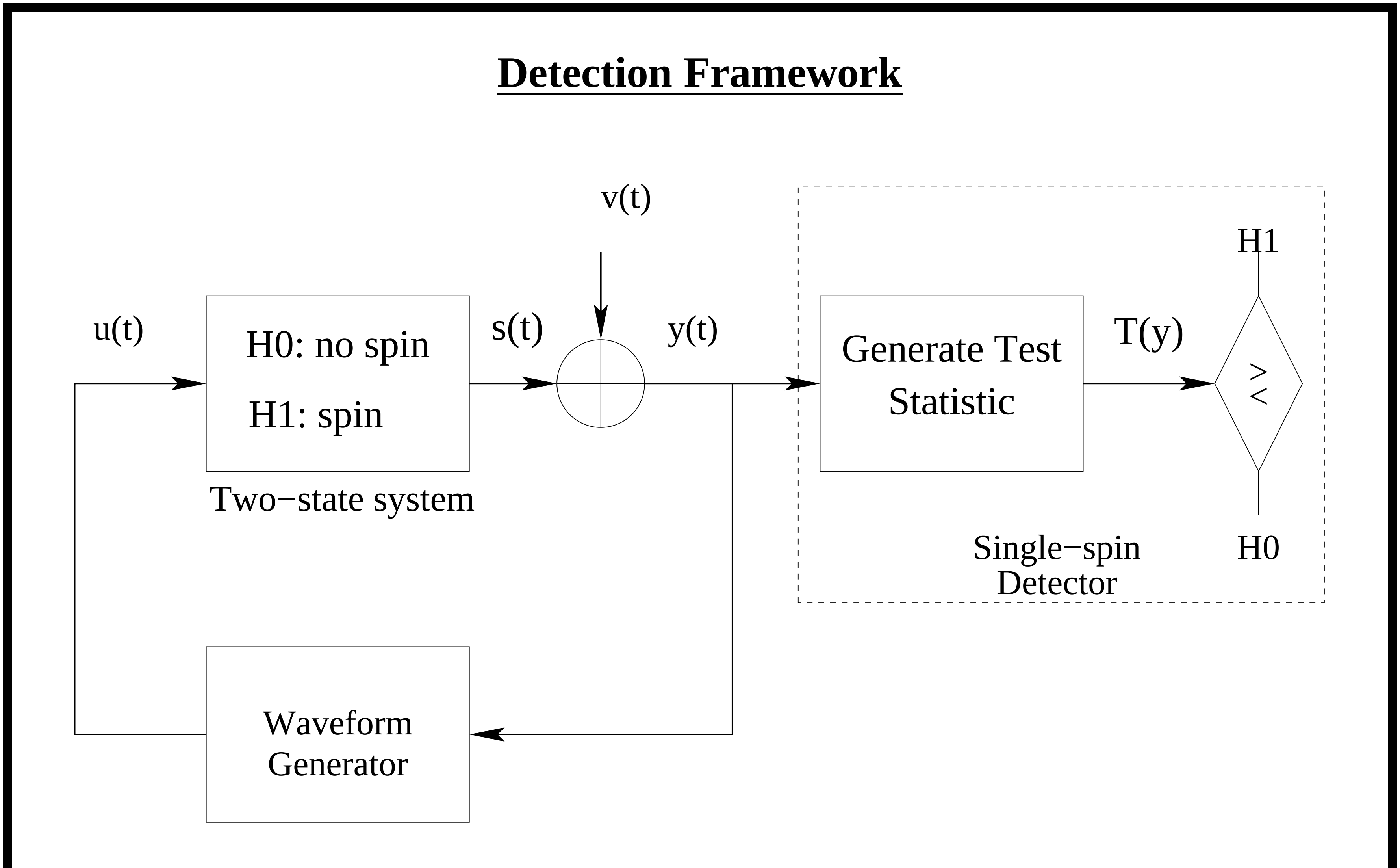


Figure 1: *Spin detection system model.*

Structure 1: Energy detector

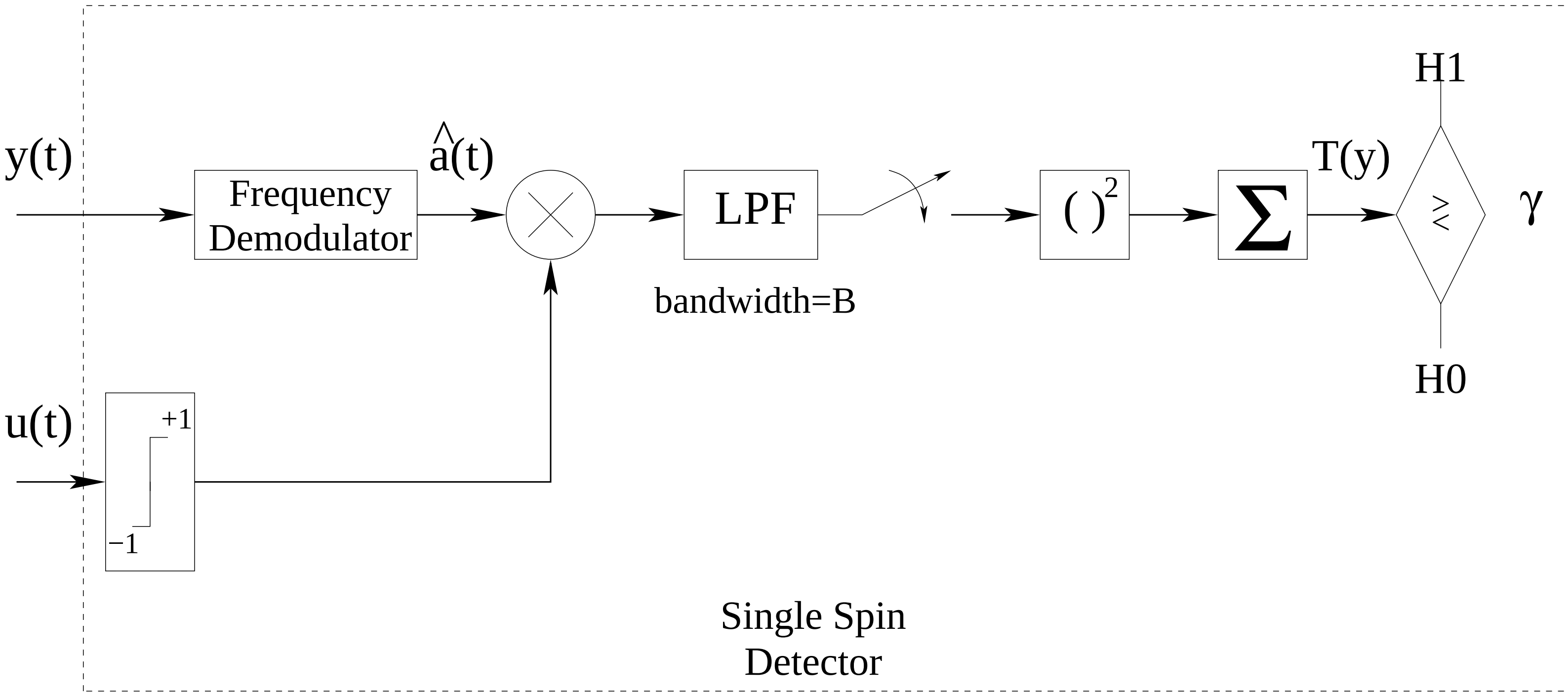


Figure 2: *Energy detector block diagram.*

- How to determine performance?

- How to determine required SNR for detection?

Energy Detector Performance

Assume:

- Random flip rate $\ll$ LPF bandwidth B

- $\hat{a}(t) = a(t) + w(t)$, $w(t)$ is zero mean Gaussian white noise of level $N_o/2$

- Detection performed over n periods of PM signal $u(t)$

Then ($\sigma^2 = BN_o$, $d =$SNR)

$$
\begin{aligned}
P_F &= P(T(y) > \gamma | H_0) \;=\; 1 - \chi_n(\gamma/\sigma^2) \;=:\; \alpha \\
P_D &= P(T(y) > \gamma | H_1) \;=\; 1 - \chi_{n,d}(\gamma/\sigma^2) \;=:\; \beta
\end{aligned}
$$

Receiver Operating Characteristic (ROC)

$$
\beta = 1 - \chi_{n,d}(\chi_n^{-1}(1-\alpha))
$$

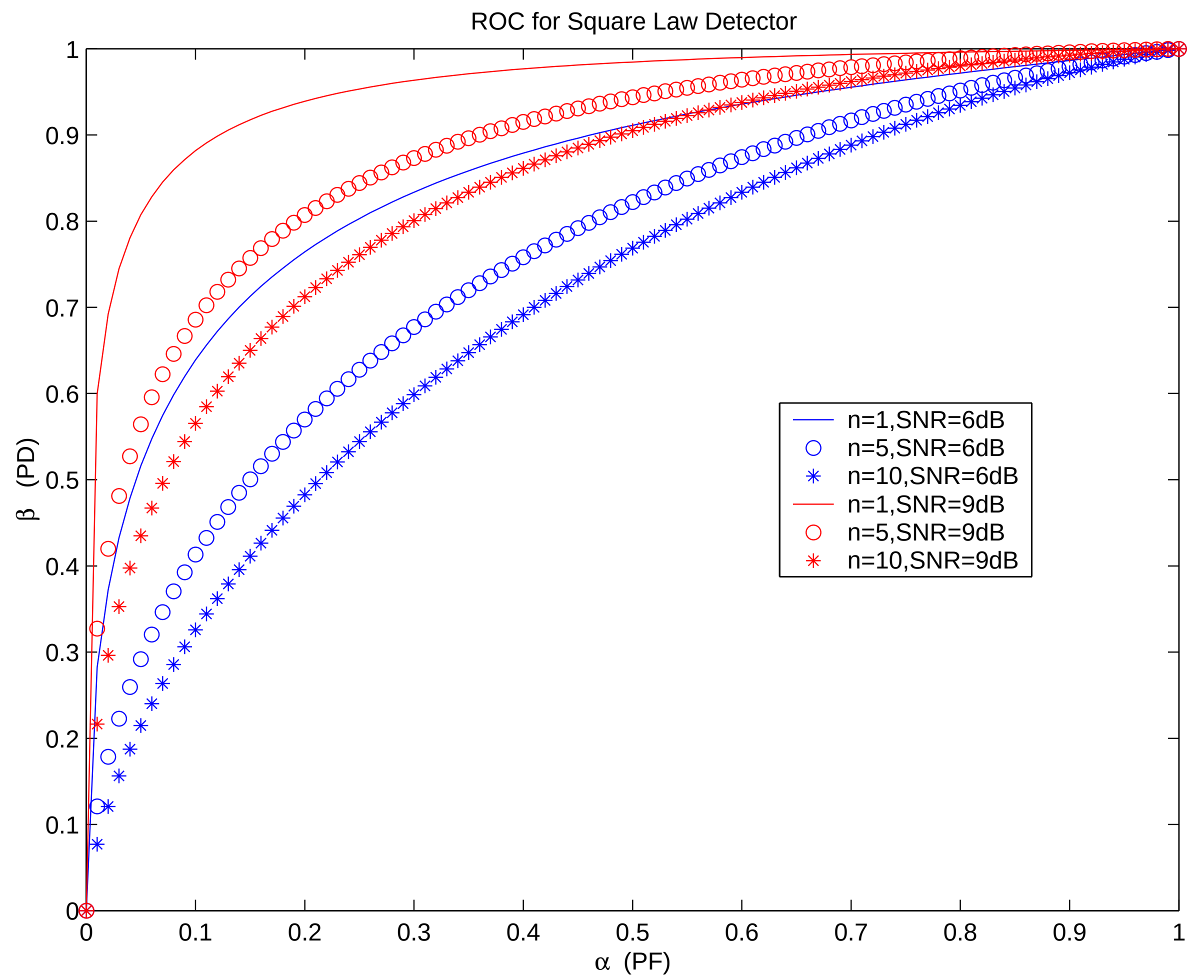


Figure 3: *ROC for two different SNR levels.*

Structure 2: GLRT

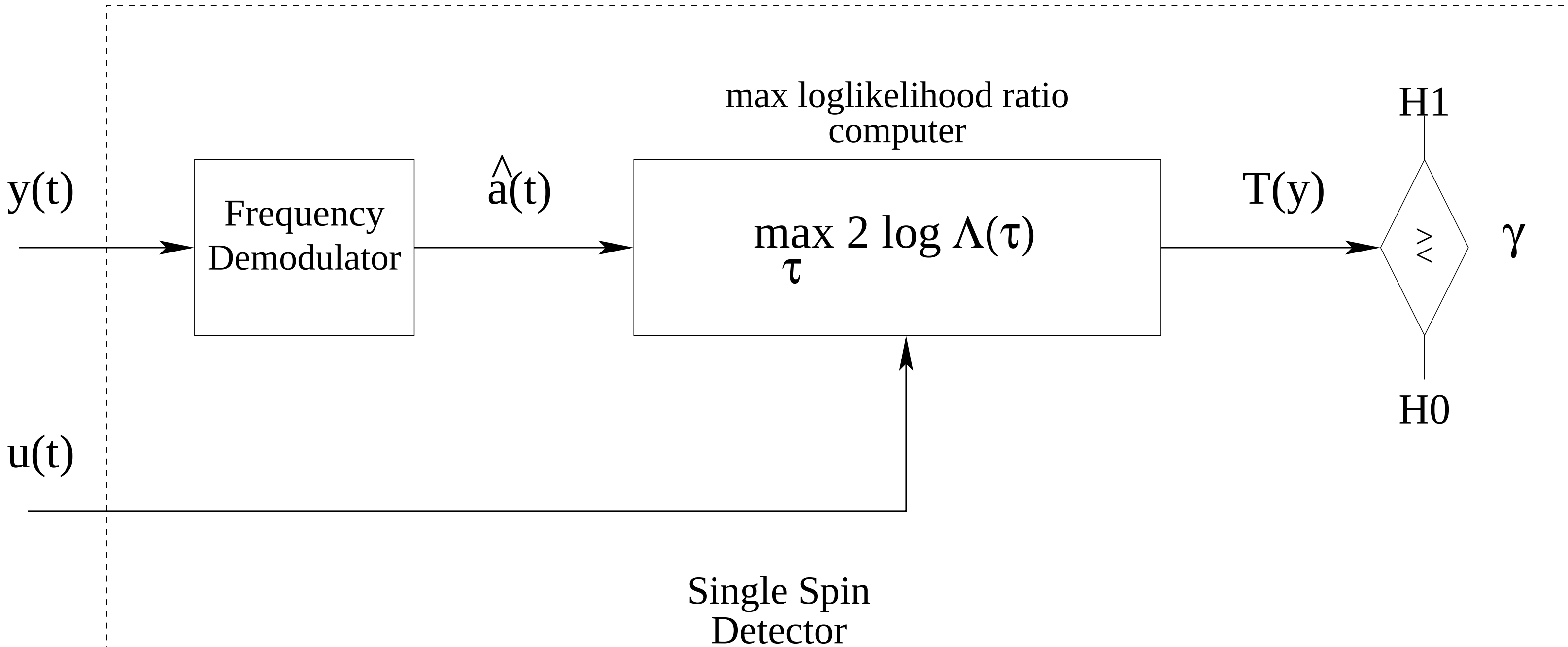


Figure 4: *Generalized likelihood ratio test under assumption of equiprobable initial spin polarity.*

$$2\log\Lambda(\tau) = 2\log\cosh\left(\sum_{i=1}^{n}(-1)^i z(\tau_i,\tau_{i-1})\right) - SNR$$

$$z(\tau_2,\tau_1) = c\int_{\tau_1}^{\tau_1} u(nT-t)\hat{a}(t)dt$$

Issues:

- ROC approximations and bounds?

- implementation complexity: multidimensional search?

- asymptotic approximations?

Structure 3: Bayes-optimal Detector

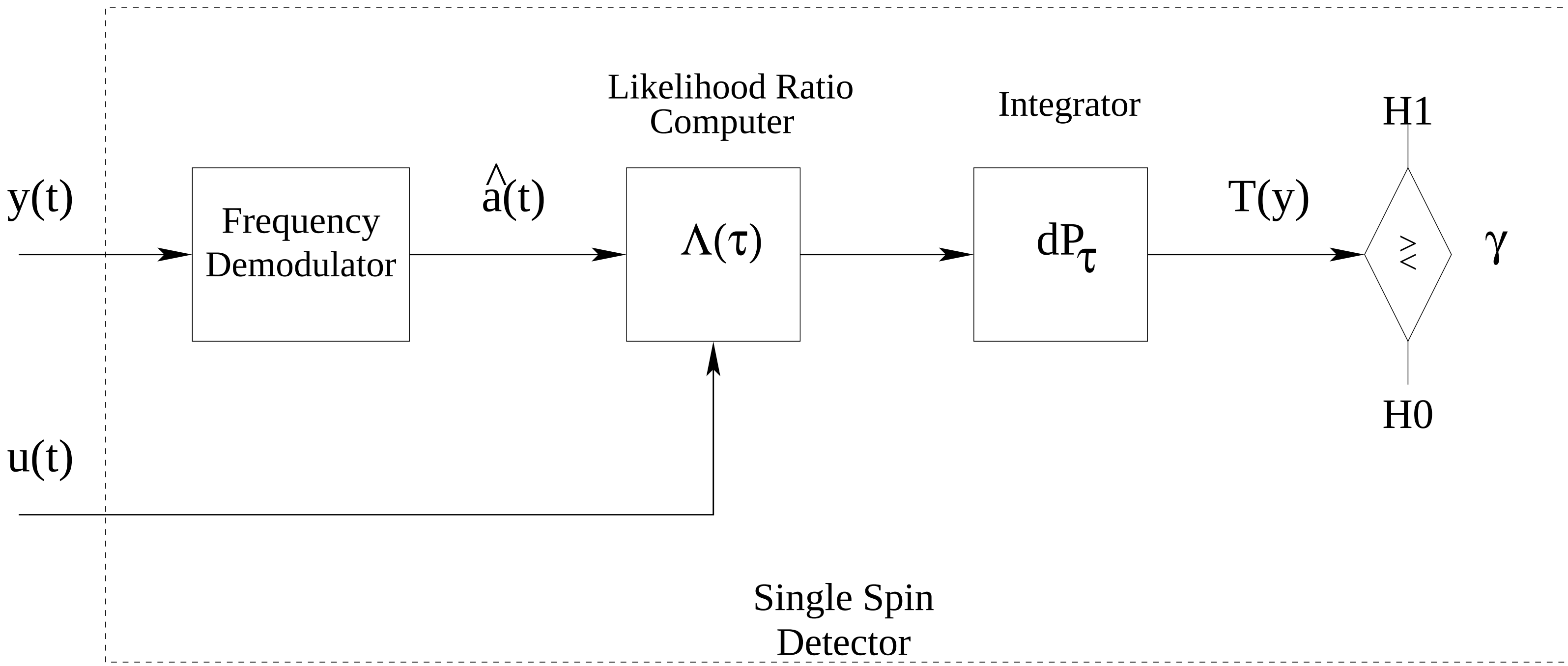


Figure 5: *Minimum P_e detector.*

Bayes detector minimizes average probability of error

$$P_e = \beta P(H_1) + \alpha P(H_0)$$

Issues:

- ROC bounds and approximations?

- implementation complexity: multiple dimensional integration?

- sensitivity to miss-specified priors?

Likelihood ratio test:

$$\Lambda(a;\underline{\theta}) = \frac{\max_{\underline{\theta}} f_{\underline{\theta}}(a \mid H_1)}{\max_{\underline{\theta}} f_{\underline{\theta}}(a \mid H_0)} > \eta$$

where $\underline{\theta}$ are random parameters (transition times, #transitions, initial phase)

f is pdf of time sampled frequency demodulator output

$$\Lambda(\hat{a};\underline{\theta}) = \operatorname*{amax}_{\underline{\theta}} \frac{\prod_{i=1}^{N} \left\{ \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{\left[\hat{a}(t_i) - a(t_i;\underline{\theta})\right]^2}{2\sigma^2} \right] \right\}}{\prod_{i=1}^{N} \left\{ \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{\left[\hat{a}(t_i)\right]^2}{2\sigma^2} \right] \right\}}$$

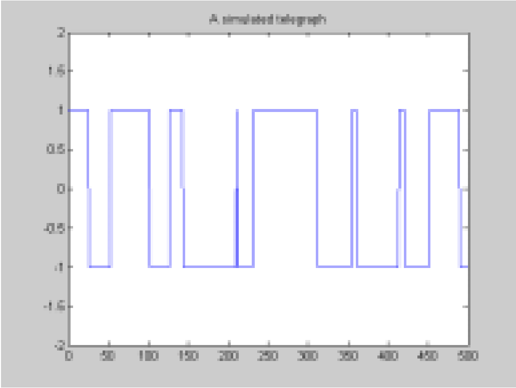
=> Equivalent test:

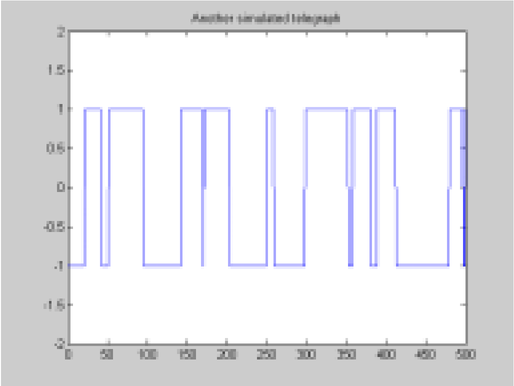
$$\frac{\operatorname*{amax}_{\underline{\theta}} \left\{ 2corr(\hat{a},a) \right\} - \overbrace{corr(a,a)}^{const.} \}}{2\sigma^2} >< \eta'$$

- **Question: How do we find θ producing maximum correlation?**

  Answer: Estimate by Markov Chain Monte Carlo (MCMC) algorithms.

- **Gibbs Sampler/particle filter**: simulate a from simulated realizations of θ: produces a random telegraph processes.

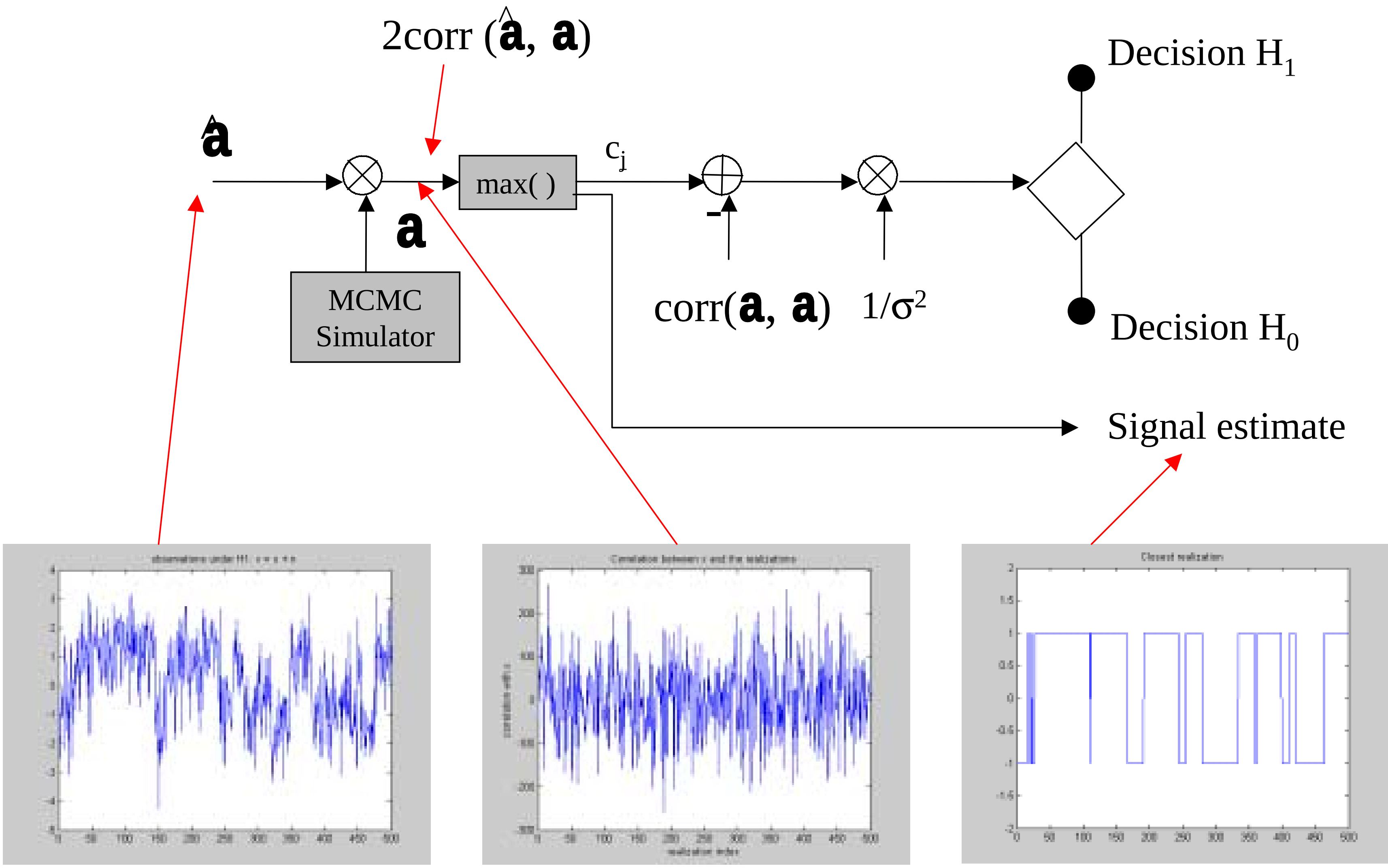




…and more!

Transition times θ drawn from a stationary Poisson process with intensity λ.

Detector Implementation:



Areas of Research

1. Determine performance and minimum SNR requirements for energy detector
2. Investigate implementation of GLR and optimal Bayes detectors
3. Find tight lower bounds and approximations on performance
4. Explore detector sensitivity/robustness to model mismatch
5. Consider more general setting of adaptive non-linear system identification
6. Integrated frequency demodulator/signal-detector
7. Signal waveform design as channel coding?
8. Single-spin tomography: reconstruction from multiple spin measurements.