Spectroscopic Detection, Fundamental Limits and System Considerations

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***Abstract*—Spectroscopic detection is the problem associated with detecting a small change in a large signal. This limit is most commonly associated with active measurements where absorption or loss is measured against frequency as in an absorption spectrometer. It results in rather different system considerations for active sensors that have been ignored or inaccurately treated in many claims of sensitivity in the submillimeter and THz regimes.**

I. Introduction And Background

The detection and quantification of absorption is a central theme in both spectroscopy and network analysis. In general it is easy to detect power and compare the power level to the noise floor of the detector to determine a carrier-to-noise floor ratio. For small signals the detector noise dominates, but in the large signal limit, noise related to the source always dominates.

The subject of sensitivity limitations for absorption spectrometers where large signals are involved was first discussed by Townes and Geschwind [1] who pointed out that the theoretical minimum detectable change in power of a large signal is proportional to the geometric mean of the noise and the signal powers:

$$\Delta P_{\min} \propto \sqrt{kT\Delta\nu P_{rx}}\,, \qquad (1)$$

where k is Boltzmann's constant, T is the receiver's physical noise temperature in the absence of signal power, $\Delta\nu$ is the detection bandwidth and P_{rx} is the received signal power.

THz spectroscopic systems have traditionally been operated in the small signal power regime, so that the minimum detectable absorbed power in a cell is determined by non-source noise terms, such as NEP of the detector. However, the improvements in sources at THz frequencies have resulted in the source noise domination. In this paper we compare the fundamental limitations of detecting small absorptions of a strong signal at THz wavelengths.

II. Results

Practical detection systems require choices be made in the sort of detector employed. Historically the emphasis has been on achieving background limited detection systems, however this is not the best optimization for a high power system.

Equation 1 states that the smallest detectable signal is at best proportional to the square root of the received power. The proportionality factor is of order unity, and we derive for the sensitivity limitation the equation:

$$\Delta P_{\min} = \sqrt{2kT\Delta\nu P_{rx}} \qquad (2)$$

Our derivation is based on the Rician probability distribution of signal detection as described by Levanon in the context of radar detection [2], and this result is in agreement with Dybdal [3]. An intuitive justification is that any power detector squares the sum of a signal and a noise voltage, $P=(Vs+Vn)^2$, so that for large signals, the cross-term $2Vs\cdot Vn \propto \sqrt{Ps\cdot Pn}$ dominates the fluctuations of the measured power.

In heterodyne detection, the system temperature, T_{sys} includes quantum noise, intrinsic mixer noise (conversion loss), as well as the thermal background noise. In most room temperature heterodyne systems T_{sys} is significantly larger than the thermal background temperature and quantum noise.

The minimum detectable power absorption of Equation 2 must also apply to the signals received by a direct detector. However, analysis of direct detectors is complicated by the fact that most are limited by internal noise or NEP, which adds an independent floor to the noise in Equation 2. As a result, the NEP becomes irrelevant at high signal levels. Direct detectors also have a less than unity quantum efficiency, γ. The performance of direct detector systems have been discussed at length by many authors, however we will adopt the formalism derived by Brown [4]. The SNR at the detector output includes the background modulation term, the background seen by the detector, the shot noise, and the intrinsic NEP.

$$SNR^2 = \frac{P_{rx}^2}{\Delta P_{\min}^2} = \frac{P_{rx}^2}{2P_{rx}kT\Delta\nu + 2(kT)^2\Delta\nu\Delta f + 2P_{rx}h\nu_c\Delta\nu + NEP^2\Delta\nu} \qquad (3)$$

Here Δf is the input bandwidth and $\Delta\nu$ is the output bandwidth. In the limit $h\nu \ll kT$, the cross-term noise will always dominate the shot noise. The shot noise limit, $h\nu \gg kT$, is equivalent to the quantum limit being substantially more than the physical temperature in a heterodyne system. The SNR with respect to the detector input can be derived by multiplying Equation 3 by the quantum efficiency.

It is useful to compare the direct detector result of Equation 3 with a heterodyne detector, where in both cases ideal detection is assumed, so that $T_{sys}\sim T$ (no mixer conversion loss or shot noise) and unity quantum efficiency. Regardless of input bandwidth and NEP all converge to the same limit.

Unfortunately real detectors can saturate, have NEPs which depend on the total load seen by the detector, and exhibit 1/f noise. This makes the cross-term fluctuation of Equation 2 difficult to measure. We developed and experimental test of Equation 3, which artificially increase the background thermal noise of a diode detector so that it dominated the intrinsic NEP. Figure 1 shows the test configuration implemented in W-band (75-110 GHz) waveguide. The thermal noise was increased by cascading two full band power amplifiers with a terminated input. The signal was coupled through a 10 dB coupler and the noise of the diode was measured with a lock-

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in noise detector at 100 kHz while power was determined from the rectified current of the diode.

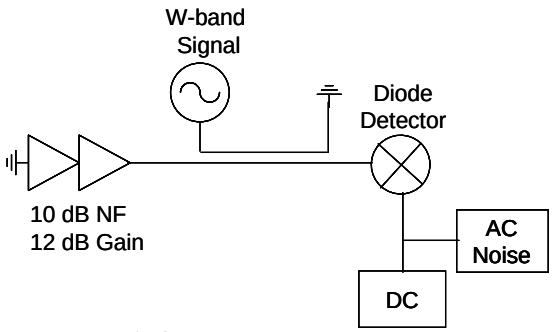

Figure 1. 75-110 GHz noise measurement system using a diode detector implemented in WR-10 waveguide.

Figure 2 shows the result of this experiment compared to a theoretical calculation assuming a 10 dB noise figure and 12 dB of average gain for each amplifier. It was also assumed that the responsivity of the detector was 1500V/W (an adjustable parameter). The figure displays the measured and theoretical excess power fluctuation of the diode response due to the cross-term of Equation 2, i.e. the excess noise beyond the diode detector's NEP. The roll off in the measured excess noise value corresponds to the onset of saturation in the diode detector. Perhaps surprisingly, saturation was already evident at 100μW. The data clearly show that, at least over about one order of magnitude in the signal power, the measured power fluctuation noise is proportional to the square root of the input signal power, as is expected from equation 3 for large powers.

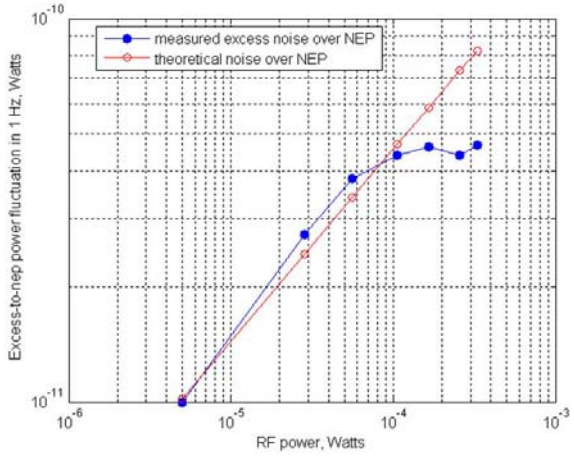

Figure 2. Noise as a function of input RF signal level showing the square root dependence and the saturation of the detector

The result is an existence proof of a noise term in detectors that is proportional to the geometric mean of the carrier power and the background thermal noise as indicated by Equation 3. We note that this noise cross-term has been frequently omitted in the analyses of THz spectroscopic systems, for example in [4] and [5]. However, the fundamental spectroscopic sensitivity limit is determined by the signal × noise cross-term of Equation 2 and will dominate all heterodyne and most direct detectors at modest power levels when hv<<kT.

III. CONCLUSIONS

The fundamental consequence of our analysis is that the weakest absorption feature that can be detected is proportional to the square root of the carrier power to the dark detector noise floor in a heterodyne system, which includes all THz time domain detectors. From fundamental principles and currently available power levels we can conclude that the state-of-the-art minimum detectable absorption is approximately one part in 10^8 in a 1 Hz bandwidth in heterodyne systems.

A useful example is the detection of Sarin gas, a nerve agent used in a terrorist attack. Sarin gas ($C_4H_{10}FO_2P$) has 140 AMU weight and a 1 Debye dipole moment. The maximum absorption coefficient is $1.55x10^{-21}$ $cm^{-1}/(molecule/cm^2)$ at 320 GHz assuming a total partition function of $5x10^6$. The Doppler width is 0.166 MHz and an assumed pressure broadening width of 4 MHz per Torr. For *in situ* detection in a 10 meter folded cell with a detectable absorption of 1 part in 10^8 in 1 second, a 250 parts per trillion or 1.5μg per m^3 gas detection limit would result. For standoff applications with 1000 meters of path, the pressure broadening smears the line width over 3 GHz increasing the detection limit by 180,000, or more than the lethal amount.

From this it can be concluded that standoff applications designed to detect biological agents or gases are not likely to generate the required sensitivity even if the instrumental problems of speckle and standing waves can be successfully addressed [6]. However, *in situ* sensing applications where Doppler limited lines are detected utilizing a widely tunable system is likely to be very competitive and potentially more reliable and flexible than any currently available gas identification technology.

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