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On the minimum detectable change of a large signal and its application to the sensitivity of microwave- and E.P.R. spectrometers

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1. INTRODUCTION.

Since the end of world war II microwave absorption and magnetic resonance techniques have been widely used and many investigators working in these fields have considered the sensitivity of their spectrometers. They derived expressions for the minimum detectable signal and the optimum absorption cell length or cavity coupling coefficient. Their results depended on the kind of spectrometers—in E.P.R. reflection or transmission type-and on the receiver systems used. Especially if for the latter a linear (amplitude sensitive) system (such as a crystal working in the linear region or a superheterodyne receiver with linear I.F. demodulation) was considered the formulae for the minimum detectable absorption coefficient of a gas or the minimum r.f. susceptibility of a paramagnetic ion and the optimum cell length or cavity coupling coefficient differed from those obtained assuming a square law (power sensitive) system (such as a bolometer or a crystal working in the quadratic region). This situation is reflected in the more recent textbooks and publications [1-4] in the field where two or more derivations are cited or given.

Now the noise voltage or noise current in a certain system is a statistical quantity. For comparison with a given signal amplitude mean square values over a certain time have to be considered. This means that the powers of the noise and the signal have to be compared. For this reason there should be just one optimum cell length or cavity coupling coefficient and one expression for the minimum sensitivity for a certain noise figure* of the receiver irrespective of whether it is of a

* As long as one is only interested in a small change of a large signal a noise figure can also be defined for nonlinear detection elements.

square law or a linear type. To remove any uncertainty about this, we have demonstrated it by explicit calculation.

2. The minimum detectable change of a large signal.

In computing the sensitivity limit in microwave and E.P.R. spectroscopy one is always facing the problem of detecting small variations in relatively large carrier signals. Gordy [5] has pointed out that in a gas spectrometer employing a superheterodyne receiver for a change ΔP of the power P at the input of the receiver the minimum detectable power change $\Delta P'$ which has to be compared to the noise power P_N is

$$\Delta \mathbf{P'} = \frac{1}{4} \frac{\Delta \mathbf{P}^2}{\mathbf{P}} \tag{1}$$

and P_N is given in the ideal case by the equipartition law: $P_N = kT \cdot \Delta \nu$ [6], where k is the Boltzmann constant, T the absolute temperature at which the receiver is operating and $\frac{1}{\Delta \nu} = \tau$, the time of observation (in a real case $\Delta \nu$ is the effective band width of the receiver, or τ is the effective time constant of the discriminator). For a non-ideal receiver $kT \cdot \Delta \nu$ is multiplied by the overall noise figure F* of the receiver or the effective overall noise temperature T* = T. F* is employed *.

We were able to show that equation (1) is not only correct for a system sensitive to signal amplitudes, i.e. a linear receiver system, but also for a system which is power sensitive, i.e. square law. The latter proof was carried out by the side-band method Townes and Geschwind [7] used first to consider the special case of a sinusoidally varying small power change. We decomposed the signal change into square waves, and by summing over all the resulting in phase side-band components, where the whole information is contained and employing the equation of completeness the relation (1) was obtained [8].

3. The sensitivity of microwave gas spectrometers.

The immediate consequence of this is that the formula for the minimum detectable absorption coefficient α_{gmin} derived by Gordy [5] for a gas spectrometer in absence of saturation and employing a superheterodyne receiver.

* To define an effective overall noise temperature T* is especially useful when masers or parametric amplifiers are employed as receivers and the cavity is at a low temperature [8].

$$\alpha_{gmin} = \frac{2}{l} \sqrt{\frac{\overline{k \,\mathrm{T}\,\Delta\,\nu\,\mathrm{F}^*}}{\mathrm{P}_0\,e^{-\alpha}c^{-l}}} \tag{2}$$

is independent of any kind of detection system and therefore valid for all gas spectrometers. P_0 is the power arriving from the generator and $l = 2/\alpha_c$ the optimum cell length which is also independent of the kind of detection system employed. α_c is the absorption coefficient of the cell.

4. The sensitivity of E.P.R. spectrometers.

With the help of equation (1) we have also computed the minimum detectable radio frequency susceptibility χ''_{min} in a magic T-reflection type and in a transmission type cavity spectrometer.

For a reflection spectrometer the power reaching the detector is

$$\mathbf{P}_{r} = \mathbf{T}_{r} \left(\beta \right) \cdot \mathbf{P}_{0} = \frac{1}{4} \left(\frac{\beta - 1}{\beta + 1} \right)^{2} \cdot \mathbf{P}_{0}$$
(3)

taking into account the double power split in the magic T (the arriving power is split and the reflected power is split again).

For the transmission type spectrometer having for optimum sensitivity equal input and output coupling coefficients β , the transmitted power P_t being equal to the power appearing at the receiver

$$P_t = T_t(\beta) \cdot P_0 = \frac{4 \beta^2}{(1+2\beta)^2} \cdot P_0$$
 (4)

The coupling coefficient β is defined in the usual way; it is the ratio between the unloaded Q (Q₀) of the cavity to the external Q (Q_e) of the cavity.

The change in power ΔP at the receiver for a change in the coupling coefficient β due to E.P.R. absorption is then given by

$$\Delta \mathbf{P} = \frac{d \mathbf{T} (\beta)}{d \beta} \Delta \beta \cdot \mathbf{P}_{\mathbf{0}} \quad \text{and} \quad \frac{\Delta \beta}{\beta} = \frac{\Delta \mathbf{Q}_{\mathbf{0}}}{\mathbf{Q}_{\mathbf{0}}}$$
(5)

After Feher [3]

$$\frac{\Delta \, Q_0}{Q_0} = \, 4 \, \pi \, \eta \, \chi^{\,\prime\prime} \, Q_0$$

where η is the filling factor of the cavity defined as

$$\eta = \frac{\int_{\text{sample}}^{\text{H}_1^2 \, d \, \phi}}{\int_{\text{cavity}}^{\text{H}_1^2 \, d \, \phi}}$$

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and H_1 is the radio frequency magnetic field component.

By combining (3) and (5) or (4) and (5) and inserting these expressions into (1), then maximising $\Delta P'$ and setting it equal to the noise power P_N we find that the minimum detectable radio frequency susceptibility χ''_{min} is *exactly* the same for both types of spectrometer. It is

$$\chi''_{min} = \frac{1}{\pi \eta Q_0} \sqrt{\frac{k \mathrm{T} \mathrm{F}^* \Delta \nu}{\mathrm{P}_0}}$$
(6)

independent of the type of spectrometer or receiver system. If therefore, a bolometer system working at low temperature could be constructed having the same effective overall noise temperature T^* as a parametric amplifier, or maser, the *same* sensitivity would be obtained with it.

We have to add that for the reflection type spectrometer the optimum coupling coefficient is found to be $\beta = 1$ and for the transmission spectrometer $\beta = \frac{1}{2}$ (independent again of the kind of detection system) which means that in both cases the external Q_e has to be equal to the internal Q_0 (the loaded Q_L has to be in both cases half the unloaded Q_0).

5. The sensitivity of microwave cavity gas spectrometers.

If we insert in equation (6) the relation $\alpha = \frac{8 \pi^2 \chi''}{\lambda_0}$ [8] where α is the absorption coefficient of a gas and λ_0 the vacuum wave length also putting $\eta = 1$ we get the minimum detectable absorption coefficient α_{min} in any cavity gas spectrometer

$$\alpha_{min} = \frac{8\pi}{\lambda_0 Q_0} \sqrt{\frac{k T \Delta v F^*}{P_0}}$$
(7)

Equation (7) can also be obtained from equation (2) in the following way: Firstly, $P_0 e^{-\alpha} c^l = P$, the power at the detector for a normal absorption cell gas spectrometer and for a transmission cavity absorption gas spectrometer the power at the detector is $P = P_0/4$. The latter equation is found by introducing the optimum coupling coefficient $\beta = \frac{1}{2}$ into equation (3). Secondly, $\alpha_g = \alpha \lambda_g / \lambda_0 = \alpha l_{eff} / 1$ where λ_g is the waveguide wave length and l_{eff} is the so-called effective absorption path of the spectrometer. For a cavity we compute [8] l_{eff} to be $l_{eff} = \frac{\lambda Q_0}{2\pi}$. Introducing the above relations into (2) gives us the previously obtained expression for α_{min} . By the double derivation of equation (7) from equation (2) and equation (6) we have also demonstrated that the expression for minimum sensitivity of a gas spectrometer can be obtained from the expression for the minimum sensitivity of an E.P.R. spectrometer and vice versa.

6. STARK AND ZEEMAN MODULATION.

We have also considered the effect of square wave or sine-modulation and lock-in detection with ground frequency response as it is usually employed in high sensitivity spectrometers for technical reasons. For spectrometers employing square wave (Stark) modulation the detectable power is $2/\pi^2$ and for sine (Zeeman) modulation it is a half that given by equation (1). This gives a factor of $\frac{\pi}{\sqrt{2}}$ for the minimum detectable signal in a microwave spectrometer employing Stark modulation and $\sqrt{2}$ in an E.P.R. spectrometer employing sinusoidal Zeeman modulation.

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