Theory of the Molecular Generator and Molecular Power Amplifier

N. G. BASOV AND A. M. PROKHOROV

P. N. Lebedev Physical Institute, Academy of Sciences, USSR

(Submitted to JETP editor Dec. 10, 1954)

J. Exptl. Theoret. Phys. (U.S.S.R.) 30, 560-563 (March, 1956)

On the basis of dispersion theory, with the effect of saturation taken into account, a theory is given of the operation of the molecular generator and of the microwave molecular power amplifier. Formulas are derived for the condition of self-excitation of the generator, and for the generated frequency and the amplitude of the steady oscillation. Other problems considered are the power amplification factor of the molecular amplifier, the bandwidth of the amplifier, and the condition for operation of the amplifier in the linear range.

1. INTRODUCTION

BY a molecular generator we mean a self-oscillatory system that uses the energy connected with transitions between different energy levels of molecules. The oscillatory circuit of a molecular generator is a cavity resonator. Through the cavity resonator is passed a molecular beam, in which there is a partial or complete absence of molecules in the lower level of the transition being used, so that such a beam is capable of radiating energy. A feedback coupling in the molecular generator is affected by the electromagnetic field of the resonator, which, acting on the dipole moments of the molecules that are passing through the resonator, causes induced emission by these molecules. In order to achieve a condition of self-excitation, the resonator must have a sufficiently high Q so that the power radiated by the molecules is greater than the power lost in the resonator and in the generator load.

The saturation effect in the induced emission constitutes the nonlinearity that determines the amplitude of the steady oscillation in the circuit of the molecular generator.

However, the molecular generator is not completely analogous to other generators with respect to the feedback coupling, since it is not a classical system; for the induced emission is an essentially quantum effect, which cannot be obtained by a classical method. In distinction from other generators, in the molecular generator the oscillatory energy is not produced in the generator circuit, but is carried into the generator circuit by the molecules of the beam, each of which must be considered to be excited by the oscillatory circuit; i.e., a molecular generator is an oscillatory system with a very large number of degrees of freedom. Therefore, the theory of operation of a molecular generator must be developed by a statistical quantum-mechanical method. In the present article this is done with the aid of dispersion theory, with the saturation effect being taken into account.[1,2]

The distinctive property of the molecular generator is the enormous stability of its frequency, for the generated frequency is little dependent on external conditions and is essentially determined by the frequency of the spectral line employed. Therefore the molecular generator can be used on the one hand as a standard of frequency, and on the other as a spectroscope of high resolving power.

If the conditions for self-excitation are not fulfilled, then the molecular generator can serve as an amplifier of microwave power with a small noise factor.

The theoretical possibility of constructing a molecular generator was pointed out in an article by us.[*,3] A report has recently appeared of a realization of such a generator.[4] It should be mentioned that in the latter work there is no theoretical consideration of the reason for the operation of such a generator.

2. THEORY OF THE MOLECULAR GENERATOR

In this section we shall obtain formulas for the generated frequency ω of a molecular generator that uses an isolated spectral line of frequency ω_r.

At the same time formulas will be obtained for the amplitude of steady oscillation of the electric field E in the generator resonator, tuned to frequency ω_0 and having quality factor Q.

The problem proposed reduces to the consideration of the behavior of a cavity resonator filled with

*The first report on the theoretical possibility of constructing a molecular generator was presented by the authors of the present article in May 1952 at the All-Union conference on radiospectroscopy.

[1]L. Landau and E. Lifshitz, *Quantum mechanics,* p. 170, (1948).

[2]R. Karplus and J. Schwinger, Phys. Rev. 73, 1020 (1948)

[3]N. G. Basov and A. M. Prokhorov, J. Exptl. Theoret. Phys. (U.S.S.R.) 27, 431 (1954).

[4]J. P. Gordon, H. J. Zeiger, and C. H. Townes, Phys. Rev. 95, 282 (1954).

a medium with negative losses in the vicinity of the frequency ω_r. In the solution of this problem we neglect the Doppler broadening of the spectral line, considering that it is always possible to choose a type of oscillation in the cavity resonator for which Doppler broadening is absent.

Let the medium be described by a complex dielectric constant

$$\varepsilon = \varepsilon' - i\varepsilon'' = 1 + 4\pi\varkappa N, \qquad (1)$$

where $\varkappa$ is the polarizability of a molecule, and N is the number density of molecules in the cavity resonator. The value of $\varkappa$, with the saturation effect taken into account, can be written in the form[1,2]

$$\varkappa = \frac{|d_{zn}^{m}|^2}{\hbar}\frac{\omega}{\omega_r} \qquad (2)$$

$$\times \frac{(\omega_r - \omega - i/\tau)(\rho_m^{(0)} - \rho_n^{(0)})}{(\omega_r - \omega)^2 + \tau^{-2} + |d_{zn}^{m}|^2|E|^2\hbar^{-2}},$$

where $|d_{zn}^{m}|^2$ is the square of the matrix element of the z-component of the dipole moment corresponding to the molecular transition between levels m and n; $\tau = l/\bar{v}$ is the mean time of transit across the resonator field, l is the length of the resonator, $\bar{v}$ is the mean speed of the molecules, $\rho_k^{(0)}$ is the probability of occurrence of molecules at level k at the moment of entry into the field of the resonator.

Let N_0 active molecules cross the cross section S of the resonator in one second:* then

$$N = N_0/S\bar{v}. \qquad (3)$$

Substituting Eq. (2) and (3) in Eq. (1), we get

$$\qquad (4)$$

$$\varepsilon' = 1 - A\gamma\frac{\omega}{\omega_r}\frac{(\omega_r - \omega)\tau}{(\omega_r - \omega)^2 + \tau^{-2} + \gamma|E|^2},$$

$$\varepsilon'' = -A\gamma\frac{\omega}{\omega_r}\frac{1}{(\omega_r - \omega)^2 + \tau^{-2} + \gamma|E|^2},$$

where

$$A = 4\pi N_0\hbar/Sl; \quad \gamma = |d_{zn}^{m}|^2/\hbar^2. \qquad (5)$$

The equation for the electric field intensity in the resonator will be written in the form

$$\frac{d^2}{dt^2}E + \frac{\omega_0}{Q}\frac{d}{dt}E + \frac{\omega_0^2}{\varepsilon}E = 0, \qquad (6)$$

where

$$E = E(x, y, z, t).$$

For simplicity we consider that E does not depend on the coordinates x, y, z of the resonator, since Eq. (4) was derived on the assumption that the field E is uniform over the cross section of the resonator. When there is a dependence of the field E on the coordinates of the cross-section, it is necessary to derive new formulas. Taking account of the fact that the magnitude of the saturation effect is different for different points within the resonator. Such a calculation cannot give anything new in principle, and our solution amounts to the introduction of a certain effective field.

We seek the stationary state in the form $E = E_0 e^{i\omega t}$. Upon substituting in Eq. (6) and setting the real and imaginary parts equal to zero, we get

$$-\omega^2 + \omega_0^2\varepsilon'/[(\varepsilon')^2 + (\varepsilon'')^2] = 0; \qquad (7)$$

$$\omega/Q + \omega_0\varepsilon''/[(\varepsilon')^2 + (\varepsilon'')^2] = 0.$$

By taking account of the expressions (4), it is possible to rewrite these equations in the form

$$\frac{Q^2}{(Q\omega/\omega_0)^2 + 1} \cdot$$

$$\qquad (8)$$

$$= 1 - A\gamma\frac{\omega}{\omega_r}\frac{(\omega_r - \omega)\tau}{(\omega_r - \omega)^2 + \tau^{-2} + \gamma|E|^2},$$

$$\frac{Q\omega_0/\omega}{(Q\omega/\omega_0)^2 + 1} \qquad (9)$$

$$= A\gamma\frac{\omega}{\omega_r}\frac{1}{(\omega_r - \omega)^2 + \tau^{-2} + \gamma|E|^2}.$$

By eliminating the amplitude of oscillation E from Eqs. (8) and (9), we get the following equation for the frequency of steady oscillation:

*By the number of active molecules we mean the difference between the numbers of molecules in the upper and lower levels of the transition under consideration.

$$\omega^3 + \omega\omega_0^2 (\omega_0\tau Q^{-1} + Q^{-2} - 1) \qquad (10)$$

$$- \omega_0^3 \omega_r \tau Q^{-1} = 0.$$

From Eq. (10) it is clear that

$$\Delta = |\omega_r - \omega| / \omega_r \ll 1. \qquad (11)$$

On solving the equation to terms of the first order in Δ, we find the generated frequency

$$\omega = \omega_r \left(1 + \frac{2Q}{\omega_0\tau} \frac{\omega_0 - \omega_r}{\omega_r} - \frac{1}{Q\omega_r\tau}\right). \qquad (12)$$

As is clear from (12), the generated frequency does not coincide with ω_r even when the resonator is exactly tuned to the frequency of the spectral line ($\omega_0 = \omega_r$). As an example, for a molecular generator with $\omega_0\tau = 2 \times 10^7$, with $Q = 1000$, and with $(\omega_0 - \omega_r)/\omega_r = 5 \times 10^{-6}$, we get $(2Q/\omega_0\tau) \times (\omega_0 - \omega_r)/\omega_r = 5 \times 10^{-10}$ and $1/Q\omega_r\tau = 5 \times 10^{-11}$.

The values quoted can be realized for a molecular generator operating on the line $J = 3$, $K = 3$ of the NH_3 molecule, i.e., such a generator can be used as an absolute standard of frequency of accuracy $\sim 10^{-9}$.

The amplitude of steady oscillation can be determined from Eq. (9). It is equal to

$$|E|^2 = \frac{1}{\gamma\tau^2} \left\{A\gamma\tau^2 \frac{1}{Q} \frac{\omega^2}{\omega_0 \omega_r} \left[\left(Q \frac{\omega}{\omega_0}\right)^2 + 1\right] \right. \qquad (13)$$

$$\left. - (\omega_r - \omega)^2 \tau^2 - 1\right\}.$$

If we consider that $\omega_0 = \omega_r \approx \omega$ and that $1/Q \ll 1$, then from (13) we get the following expression for the limit of self-excitation of the generator:

$$A\gamma\tau^2 Q > 1 \quad \text{or} \quad \frac{4\pi N_0}{Sl\hbar} |d_{zn}^m|^2 Q\tau^2 > 1. \qquad (14)$$

The expression (14) was obtained by us earlier in Ref. 3. If $A\gamma\tau^2 Q \gg 1$, , then the amplitude of steady oscillation takes the form

$$|E|^2 = (4\pi N_0 \hbar\omega_r / Sl) Q, \qquad (15)$$

in this case the molecular beam radiates to the resonator the maximum possible power

$$W_{\max} = \frac{1}{2} N_0 \hbar\omega_r. \qquad (16)$$

3. THE MOLECULAR MICROWAVE POWER AMPLIFIER

If the condition for self-excitation in a molecular generator is not satisfied, then such an apparatus can be used as an amplifier of microwave power. This apparatus is analogous to a regenerative receiver. A molecular generator possesses a small noise factor.

We shall find the power amplification factor of such an amplifier. The molecular amplifier is described by the same equations as the molecular generator, except that on the right side of Eq. (6) it is necessary to add the external force, related to the power being amplified:

$$\frac{d^2}{dt^2} E + \frac{\omega_0}{Q} \frac{d}{dt} E + \frac{\omega_0^2}{\varepsilon} E = \omega^2 B e^{i\omega t}. \qquad (17)$$

The amplitude of the external force B is determined by the power input W_i to the amplifier resonator. We can represent by W_0 the power output from the amplifier; then the power amplification factor of the amplifier is

$$K = W_0 / W_i \qquad (18)$$

In the absence of the molecular beam, K is the coefficient of power transmission through the resonator.

To find the amplification (transmission) factor, we shall calculate the field in the resonator in two cases: in the presence of the molecular beam in the resonator, E_1, and in its absence E_2. Then the power amplification factor will be equal to the ratio of the squares of the field in the resonator in these two cases, multiplied by the coefficient of transmission through the resonator K_0 in the absence of the molecular beam:

$$K = K_0 (E_1 / E_2)^2. \qquad (19)$$

From Eq. (17) we get the following value of E_1:

$$|E_1|^2 = B^2 \left\{\left[\left(\frac{\omega_0}{\omega}\right)^2 \frac{\varepsilon'}{(\varepsilon')^2 + (\varepsilon'')^2} - 1\right]^2 \right. \qquad (20)$$

$$\left. + \left[\left(\frac{\omega_0}{\omega}\right)^2 \frac{\varepsilon''}{(\varepsilon')^2 + (\varepsilon'')^2} + \frac{1}{Q} \frac{\omega_0}{\omega}\right]^2\right\}^{-1}.$$

We get E_2 from (20) by setting $\epsilon' = 1$, $\epsilon'' = 0$.

At resonance, $\omega_0 = \omega_r = \omega$, the amplification

factor has its maximum value. It is equal to

$$K_m = K_0 / (1 - A\gamma\tau^2 Q)^2. \qquad (21)$$

From (21) it is possible to estimate the bandwidth Δ of the amplifier. We shall define the bandwidth of the amplifier as the amount of detuning of the frequency, with respect to the resonance frequency, for which the amplified power is diminished by a factor two. For $K < Q$,

$$\Delta^2 = (1/\tau^2) K_0 / K_m. \qquad (22)$$

Eq. (22) shows that the bandwidth of the amplifier decreases with increase of the amplification factor of the amplifier. This also takes place in an ordinary regenerative receiver.

In order that the amplifier may operate in the linear range (far below saturation), the following condition must be satisfied:

$$\gamma\tau^2 |E_1|^2 \ll 1. \qquad (/)$$

Translated by W. F. Brown, Jr.
100