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[30]It would be possible to introduce different kernels for the two states $|a\rangle$ and $|b\rangle$ by assuming that the scattering depends on the state of the atom. We do, however, assume the transational degree of freedom to be uncoupled with the internal state of the atom and this assumption allows only one function.

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$$\overline{\exp(-i\eta)}=\overline{\cos\,\eta}-i\,\overline{\sin\eta}.$$

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Linewidths of a Gaussian Broadband Signal in a Saturated Two-Level System*

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The spectral power distribution of a broadband maser signal that is saturating a two-level system is derived using stationary Gaussian statistics for the electric fields and assuming the bandwidth is large compared to the homogeneous linewidths of the two levels. The results are applied to travelling-wave amplifiers of this type, the cosmic OH and H_2O masers, to obtain the saturated maser output intensity and linewidth as a function of amplifier length.

I. INTRODUCTION

The spectral distribution of steady-state broadband maser emission at any point in a saturated amplifier has not been adequately presented, even for a two-level system, in previous work.[1-3] For reasons of tractability, such a power spectrum is derived here based on the approximations that antiresonance and second-harmonic terms can be neglected, that the electric fields have nearly stationary Gaussian statistics, and that the bandwidth is large compared to the homogeneous (natural, collision, or pumping) linewidths of the two levels. A multiple-level system, appropriate to the analysis of the competition between modes having orthogonal polarization, can also be handled by considering coupled equations for the power spectrum of the two modes. However, we consider here just two levels which are connected by an electric dipole moment and a microwave field of a given circular or linear polarization and Zeeman transition. Nevertheless, these conditions are probably appropriate for the cosmic OH and H_2O masers,[3,4] whose output characteristics we will deal with below.

II. SPECTRAL POWER DISTRIBUTION – SIX CASES

The equations of motion for the two-level (a and b) density matrix (in the interaction representation) are as follows:

$$\dot{\rho}_{aa}(t)=i^{-1}[V_{ab}(t)\,\rho_{ba}(t)-\rho_{ab}(t)\,V_{ba}(t)]-\Gamma_{aa}\rho_{aa}(t)+\Lambda_{aa}\,,$$

$$\dot{\rho}_{ab}(t)=i^{-1}V_{ab}(t)[\rho_{bb}(t)-\rho_{aa}(t)]-\Gamma_{ab}\rho_{ab}(t)\,, \qquad (1)$$

$$\dot{\rho}_{bb}(t)=i^{-1}[V_{ba}(t)\,\rho_{ab}(t)-\rho_{ba}(t)\,V_{ab}(t)]-\Gamma_{bb}\rho_{bb}(t)+\Lambda_{bb}\,,$$

$$\rho_{ba}(t)=\rho^*_{ab}(t)\,,$$

where the damping factors $\Gamma_{ij}=\frac{1}{2}(\Gamma_{ii}+\Gamma_{jj})$ give the net rates out of the states, and the production rates Λ_{aa} and Λ_{bb} give the net rates into the states. The interaction is given by

$$V_{ab}(t)=\vec{\mu}_{ab}\,e^{-i\omega_{ba}t}\cdot\vec{\mathrm{E}}(t)/\hbar\,, \qquad (2)$$

where $\vec{\mu}_{ab}$ is the electric-dipole-moment matrix element and the electric field is

$$\vec{\mathrm{E}}(t)=\tfrac{1}{2}\int_{-\infty}^{\infty}d\omega\,\vec{\mathrm{E}}(\omega)\,e^{-i\omega t}=\tfrac{1}{2}\int_{0}^{\infty}d\omega\,[\,\vec{\mathrm{E}}(\omega)\,e^{-i\omega t}+\vec{\mathrm{E}}^{+}(\omega)e^{i\omega t}\,]\,. \qquad (3)$$

The polarization (electric dipole moment per unit volume) of the medium has a Fourier component $\vec{\mathcal{P}}(\omega)$ at frequency ω,

$$\vec{\mathcal{P}}(\omega)=\int_{-\infty}^{\infty}(dt/2\pi)\,e^{i\omega t}\,\tfrac{1}{2}\,[\,\vec{\mu}_{ba}\,e^{i\omega_{ba}t}\rho_{ab}(t)+\vec{\mu}_{ab}\,e^{-i\omega_{ba}t}\rho_{ba}(t)\,]\,, \qquad (4)$$

where

$$\rho_{ab}(t)=i^{-1}\int_{-\infty}^{t}V_{ab}(t')\,[\rho_{bb}(t')-\rho_{aa}(t')]e^{-\Gamma_{ab}(t-t')}dt'$$
$$=i^{-2}\int_{-\infty}^{t}dt'\int_{-\infty}^{t'}dt''\,V_{ab}(t')(e^{-\Gamma_{bb}(t'-t'')}+e^{-\Gamma_{aa}(t'-t'')})\times[V_{ba}(t'')\rho_{ab}(t'')-V_{ab}(t'')\rho_{ba}(t'')]e^{-\Gamma_{ab}(t-t')}$$
$$+i^{-1}\int_{-\infty}^{t}V_{ab}(t')e^{-\Gamma_{ab}(t-t')}\,dt'\,\Delta\rho\,. \qquad (5)$$

Here, $\Delta\rho=\Lambda_{bb}/\Gamma_{bb}-\Lambda_{aa}/\Gamma_{aa}$ is the steady-state population inversion in the absence of saturation.

If we consider pumping only between the two levels without any destruction or formation of the molecules, then we may write $\Lambda_{aa}=W_{ab}\rho_{bb}$ and $\Lambda_{bb}=W_{ba}\rho_{aa}$, and then we replace each Γ_{aa} and Γ_{bb} in all the formulas given below by $W_{ab}+W_{ba}$, where W_{ab} and W_{ba} are the net pump and collision rates from b to a and from a to b, respectively.

The average power output per unit volume at frequency ω is obtained from the time or ensemble average of the product of the polarization and the microwave field, i.e., the power density is $-\omega\,\mathrm{Im}\langle\vec{\mathcal{P}}(\omega)\cdot\vec{\mathrm{E}}(\omega)\rangle$. If the increase of intensity occurs over distances that are large compared with the wavelength, then, from the Maxwell equations,

$$d\langle\vec{\mathrm{E}}^{+}(\omega)\cdot\vec{\mathrm{E}}(\omega)\rangle/ds\simeq-8\pi\omega\,\mathrm{Im}\langle\vec{\mathcal{P}}(\omega)\cdot\vec{\mathrm{E}}(\omega)\rangle/c\,,$$

where ds is an element of distance along the ray path. The Fourier component of the off-diagonal density-matrix element in $\vec{\mathcal{P}}(\omega)$ is obtained from Eq. (5) as

$$\rho_{ab}(\Omega)\equiv\int_{-\infty}^{\infty}\rho_{ab}(t)\,e^{i\Omega t}\,(dt/2\pi)\simeq(\mu_{ab}/2\hbar i)\,(\Gamma_{ab}-i\Omega)^{-1}\,\Delta\rho\,E^{+}(\omega_{ba}-\Omega)$$
$$-(|\mu_{ab}|^2/4\hbar^2)(\Gamma_{ab}-i\Omega)^{-1}\int\int d\omega_2d\omega_1K_{ab}(\omega_{ba}-\omega_2-\Omega)\,E^{+}(\omega_2)$$
$$\times[\mu_{ba}E(\omega_1)\,\rho_{ab}(\Omega+\omega_2-\omega_1)-\mu_{ab}E^{+}(\omega_1)\,\rho_{ba}(\Omega+\omega_2+\omega_1-2\,\omega_{ba})]\,, \qquad (6)$$

where the sharply-resonant kernel

$$K_{ab}(\omega)\equiv(\Gamma_{aa}+i\omega)^{-1}+(\Gamma_{bb}+i\omega)^{-1}\,.$$

In order to obtain the power output at frequency ω, we will need ω times the imaginary part of the complex quantity

$$\langle \vec{\mathcal{P}}(\omega)\cdot\vec{E}(\omega')\rangle = \mu_{ba}\langle \rho_{ab}(\omega_{ba}-\omega)E(\omega')\rangle ,$$

which we obtain from the above expression for ρ_{ab}, evaluated at $\Omega=\omega_{ba}-\omega$:

$$\mu_{ba}\langle \rho_{ab}(\omega_{ba}-\omega)E(\omega')\rangle \simeq (|\mu_{ab}|^2/2\hbar i)[\Gamma_{ab}+i(\omega-\omega_{ba})]^{-1}\Delta\rho\langle E^+(\omega)E(\omega')\rangle - (|\mu_{ab}|^2/4\hbar^2)[\Gamma_{ab}+i(\omega-\omega_{ba})]^{-1}$$
$$\times\int_0^\infty d\omega_2 K_{ab}(\omega-\omega_2)\langle E^+(\omega_2)E(\omega')\rangle\int_0^\infty d\omega_1[\mu_{ba}\langle\rho_{ab}(\omega_{ba}-\omega+\omega_2-\omega_1)E(\omega_1)\rangle$$
$$-\mu_{ab}\langle\rho_{ba}(\omega_1+\omega_2-\omega-\omega_{ba})E^+(\omega_1)\rangle] - (|\mu_{ab}|^2/4\hbar^2)[\Gamma_{ab}+i(\omega-\omega_{ba})]^{-1}$$
$$\times\int_0^\infty\int_0^\infty d\omega_2 d\omega_1 K_{ab}(\omega-\omega_2)[\langle E^+(\omega_2)E(\omega_1)\rangle\langle\rho_{ab}(\omega_{ba}-\omega+\omega_2-\omega_1)E(\omega')\rangle\mu_{ba}$$
$$-\mu_{ab}\langle E^+(\omega_1)E(\omega')\rangle\langle\rho_{ba}(\omega_1+\omega_2-\omega-\omega_{ba})E^+(\omega_2)\rangle] , \quad (7)$$

which has been averaged with one pair-wise electric field correlation function factored out, as allowed by Gaussian statistics. We have neglected the correlation of E with E or E^+ with E^+ or of ρ_{ba} with E, etc., since we are ignoring the small second-harmonic generation and antiresonance terms. We also assume stationary statistics, so that $\langle E^+(\omega)E(\omega')\rangle = F(\omega)\delta(\omega-\omega')$. That is, only fields of the same frequency are correlated. Note that the mean-square intensity $I(\omega)=F(\omega)c/8\pi$. Then we may define $p(\omega)$ such that

$$\mu_{ba}\langle\rho_{ab}(\omega_{ba}-\omega)E(\omega')\rangle \equiv p(\omega)\delta(\omega-\omega') .$$

Therefore, from the previous equation, we obtain the useful integral equation

$$p(\omega)\simeq[W(\omega)\hbar/\pi i][\Gamma_{ab}+i(\omega-\omega_{ba})]^{-1}\Delta\rho$$
$$-[\Gamma_{ab}+i(\omega-\omega_{ba})]^{-1}K_{ab}(0)[W(\omega)/2\pi]$$
$$\times\int_0^\infty d\omega_1[p(\omega_1)-p^+(\omega_1)]$$
$$-[\Gamma_{ab}+i(\omega-\omega_{ba})]^{-1}\int_0^\infty(d\omega_2/2\pi)K_{ab}(\omega-\omega_2)$$
$$\times[W(\omega_2)p(\omega)-p^+(\omega_2)W(\omega)] , \quad (8)$$

where

$$W(\omega)=2\pi|\mu_{ab}|^2F(\omega)/4\hbar^2 \quad (9)$$

is the usual induced transition rate that is proportional to the intensity. A similar equation for $p^+(\omega)$ is obtained by taking the complex conjugate of Eq. (8). We now consider cases A–F which are distinguished by whether the line broadening is homogeneous or inhomogeneous, whether the signal is narrow or broadband, and whether the saturation is moderate or extreme.

A. Homogeneous Broadening and Quasimonochromatic Signal

If the Doppler (inhomogeneous) broadening is negligible compared to the (homogeneous) broadening owing to collisions or pumping, and if the signal bandwidth is also small compared to the homogeneous linewidth, then we have the simplest case for applying the Eq. (8).

For the quasimonochromatic case, for which $W(\omega)$ is sharper in frequency than Γ, we have

$$\left[\Gamma_{ab}+i(\omega-\omega_{ba})+\frac{W}{2\pi}\left(\frac{1}{\Gamma_{aa}}+\frac{1}{\Gamma_{bb}}\right)\right]p(\omega)$$
$$\simeq\frac{W(\omega)\hbar\Delta\rho_{\text{sat}}}{\pi i}+\left(\frac{1}{\Gamma_{aa}}+\frac{1}{\Gamma_{bb}}\right)\frac{W}{2\pi}p^+(\omega) ,$$

where

$$W=\int_0^\infty W(\omega)d\omega .$$

So that, upon taking real and imaginary parts of both sides of the above equation, we have

$$\Gamma_{ab}P'(\omega)-(\omega-\omega_{ba})P''(\omega)=0 ,$$

$$(\omega-\omega_{ba})P'(\omega)+\left[\Gamma_{ab}+\frac{W}{\pi}\left(\frac{1}{\Gamma_{aa}}+\frac{1}{\Gamma_{bb}}\right)\right]P''(\omega)$$
$$=\frac{-W(\omega)\hbar\Delta\rho_{\text{sat}}}{\pi} ,$$

where $P'=\text{Re}\,p$ and $P''=\text{Im}\,p$. Therefore, we have

$$-P''(\omega)=\frac{\Gamma_{ab}W(\omega)\hbar\Delta\rho_{\text{sat}}\pi^{-1}}{(\omega-\omega_{ba})^2+\Gamma_{ab}^2+\Gamma_{ab}W[(1/\Gamma_{aa})+(1/\Gamma_{bb})]\pi^{-1}} ,$$

where the saturated population inversion is

$$\Delta\rho_{\text{sat}}=\Delta\rho+\frac{1}{\hbar}\left(\frac{1}{\Gamma_{aa}}+\frac{1}{\Gamma_{bb}}\right)\int_0^\infty d\omega_1 P''(\omega_1)=\Delta\rho-\frac{\Gamma_{ab}W\Delta\rho_{\text{sat}}[(1/\Gamma_{aa})+(1/\Gamma_{bb})]\pi^{-1}}{(\omega-\omega_{ba})^2+\Gamma_{ab}^2+\Gamma_{ab}W[(1/\Gamma_{aa})+(1/\Gamma_{bb})]\pi^{-1}} ,$$

or

$\Delta\rho/\Delta\rho_{\mathrm{sat}}$

$$= 1 + \left[(\omega - \omega_{ba})^2 + \Gamma_{ab}^2 + \Gamma_{ab} W \left(\frac{1}{\Gamma_{aa}} + \frac{1}{\Gamma_{bb}} \right) \pi^{-1} \right]^{-1}$$

$$\times \Gamma_{ab} W \left(\frac{1}{\Gamma_{aa}} + \frac{1}{\Gamma_{bb}} \right) \pi^{-1} .$$

Therefore, the spectral power distribution is

$-\omega P''(\omega)$

$$= \frac{\Gamma_{ab} W(\omega) \hbar \omega \Delta\rho \pi^{-1}}{(\omega - \omega_{ba})^2 + \Gamma_{ab}^2 + 2\Gamma_{ab} W[(1/\Gamma_{aa}) + (1/\Gamma_{bb})]\pi^{-1}} . \quad (10)$$

The linewidth $[\Gamma_{ab}^2 + 2\Gamma_{ab} W(\Gamma_{aa}^{-1} + \Gamma_{bb}^{-1})\pi^{-1}]^{1/2}$ compares with $[\Gamma_{ab}^2 + \Gamma_{ab} W(\Gamma_{aa}^{-1} + \Gamma_{bb}^{-1})\pi^{-1}]^{1/2}$ for the truly monochromatic case for which Eqs. (7) and (8) would not have the last group of terms, to avoid redundancy when $\langle \cdots \rangle$ is omitted and amplitude fluctuations vanish.

B. Homogeneous Broadening, Broadband Signal, and Moderate Saturation

Though $W(\omega)$ may be comparable to or greater than Γ_{aa} and Γ_{bb}, for this case we have $W(\omega) \ll \delta\omega$, the spectral half-width of $W(\omega)$. As can be verified *a posteriori*, the last integral in Eq. (8), involving $\int d\omega_2 K_{ab}(\omega - \omega_2) p^+(\omega_2)$, may then be neglected. This quantity is roughly a factor $dW(\omega)/d\omega$ smaller than the terms that we will keep. This integral does not vanish, because $p^+(z)$ is not analytic in the upper half-plane $\mathrm{Im}\, z > 0$, because $W(z)$ is not, since analyticity would imply a vanishing intensity for $t < 0$.

We then have, from Eq. (8), according to procedures similar to those used above, and with

$$\int d\omega_2 \, K_{ab}(\omega - \omega_2) \, W(\omega_2)/2\pi \simeq W(\omega) + i\Omega(\omega) ,$$

where $\Omega(\omega) = \int' d\omega_2 W(\omega_2)/(\omega_2 - \omega)\pi$ (here $\int'$ is the Cauchy principal-value integral),

$$p(\omega) \simeq W(\omega) \hbar \Delta\rho_{\mathrm{sat}} (\pi i)^{-1} [\Gamma_{ab} + W(\omega) + i(\omega - \tilde{\omega}_{ba})]^{-1} ,$$

where

$$\Delta\rho_{\mathrm{sat}} = \Delta\rho [1 + K_{ab}(0) G]^{-1}, \quad \tilde{\omega}_{ba} = \omega_{ba} - \Omega(\omega) ,$$

and

$$G = \int \frac{W(\omega)[\Gamma_{ab} + W(\omega)] d\omega/\pi}{(\omega - \tilde{\omega}_{ba})^2 + [\Gamma_{ab} + W(\omega)]^2}$$

$$\simeq W(\omega_{ba}) \quad \text{for } W(\omega) \ll \delta\omega .$$

Then, from the imaginary part of the above equation for $p(\omega)$, we have

$$-\omega P''(\omega) \simeq \frac{W(\omega) \hbar \omega \Delta\rho [\Gamma_{ab} + W(\omega)] \pi^{-1}}{(\omega - \tilde{\omega}_{ba})^2 + [\Gamma_{ab} + W(\omega)]^2}$$

$$\times [1 + (\Gamma_{aa}^{-1} + \Gamma_{bb}^{-1}) W(\omega_{ba})]^{-1} . \quad (11)$$

This result merely shows the effect of the added damping rate $W(\omega)$ on the lifetimes of the levels. The saturation of the population inversion by the factor $[1 + (\Gamma_{aa}^{-1} + \Gamma_{bb}^{-1}) W(\omega_{ba})]^{-1}$ can be obtained from the rate equations for the steady-state populations under an induced transition rate $W(\omega_{ba})$. We note that despite the line broadening by an added amount $W(\omega)$, the value of $-\int d\omega\, \omega P''(\omega)$, the total power output, is the same as expected from the steady-state transfer of populations, and not from Raman-type saturation effects.[2,5] The frequency shift $-\Omega(\omega)$ is antisymmetric when $W(\omega)$ is symmetric about line center ω_{ba}.

C. Homogeneous Broadening, Broadband Signal, and Extreme Saturation

One can approximate

$W(\omega) \int d\omega_2 \, K_{ab}(\omega - \omega_2) p^+(\omega_2)/2\pi$

by

$p^+(\omega) \int d\omega_2 \, K_{ab}(\omega - \omega_2) \, W(\omega_2)/2\pi$

in the last integral of Eq. (8), since $p^+(\omega)$ is proportional to $W(\omega)$, and since the width of $p^+(\omega)/W(\omega)$ is much greater than Γ_{aa} of Γ_{bb} for this case. We will avoid the complicated transition from the preceding case to this one, when the approximate linewidth goes from $\Gamma_{ab} + W(\omega_{ba})$ to $[\Gamma_{ab}^2 + 2W(\omega_{ba})\Gamma_{ab}]^{1/2} \gg \delta\omega$. Then, from Eq. (8), we have

$P''(\omega)$

$$\simeq \frac{-W(\omega) g(\omega - \omega_{ba}) [\Delta\rho \hbar + K_{ab}(0) \int d\omega_1 \, P''(\omega_1)]}{1 + 2\int d\omega_2 \, W(\omega_2) L(\omega, \omega_2)} ,$$

where

$$L(\omega, \omega_2) = \mathrm{Re}\{[\Gamma_{ab} + i(\omega - \omega_{ba})]^{-1} K_{ab}(\omega - \omega_2)/2\pi\} .$$

Here, we have $g(\omega) = \mathrm{Re}[\Gamma_{ab} + i\omega]^{-1}/\pi$. Then, integrating both sides of this equation over ω and solving for $\int P''(\omega) d\omega$ yields

$$\int P''(\omega) d\omega \simeq -\hbar \Delta\rho G [1 + K_{ab}(0) G]^{-1} ,$$

where

$$G \equiv \int \frac{W(\omega) g(\omega - \omega_{ba}) d\omega}{1 + 2\int d\omega_2 \, W(\omega_2) L(\omega, \omega_2)} .$$

If we approximate $L(\omega, \omega_2)$ by

$L(\omega, \omega_2)$

$$\simeq g(\omega - \omega_{ab}) \frac{1}{2} \left(\frac{\Gamma_{aa}}{\Gamma_{aa}^2 + (\omega - \omega_2)^2} + \frac{\Gamma_{bb}}{\Gamma_{bb}^2 + (\omega - \omega_2)^2} \right) ,$$

we obtain for $P''(\omega)$, provided $\delta\omega \gg \Gamma_{aa}$ and Γ_{bb},

$$P''(\omega) \simeq \frac{-W(\omega) g(\omega - \omega_{ba}) \hbar \Delta\rho_{\mathrm{sat}}}{1 + g(\omega - \omega_{ba}) 2\pi \, W(\omega)}$$

$$= \frac{-W(\omega)\Gamma_{ab} \hbar \Delta\rho_{\mathrm{sat}}/\pi}{(\omega - \omega_{ba})^2 + \Gamma_{ab}^2 + 2W(\omega)\Gamma_{ab}} , \quad (12)$$

where $\Delta\rho_{sat} \equiv \Delta\rho[1 + K_{ab}(0)G]^{-1}$ and

$$G \simeq \int \frac{W(\omega)g(\omega - \omega_{ba})\,d\omega}{1 + 2g(\omega - \omega_{ba})\,W(\omega)}$$

$$= \int_0^\infty \frac{W(\omega)\,d\omega\,\Gamma_{ab}/\pi}{(\omega - \omega_{ba})^2 + 2\,\Gamma_{ab}\,W(\omega) + \Gamma_{ab}^2}\,.$$

All these results apply only when $[\Gamma_{ab}^2 + 2W(\omega_{ba})\Gamma_{ab}]^{1/2} \gg \delta\omega \gg \Gamma_{aa}, \Gamma_{bb}$. When $\delta\omega \ll \Gamma_{aa}, \Gamma_{bb}$, the quasimonochromatic case applies.

D. Inhomogeneous Broadening and Quasimonochromatic Signal

With inhomogeneous broadening (e.g., due to thermal Doppler effects) we replace ω_{ba} by $\omega_{ba}(v) \equiv \omega_{ba}(1 + v/c)$. We assign a probability $g_D(v)\,dv$ to the differential number of molecules with this velocity, $\int g_D(v)\,dv = 1$. The Doppler width $\delta\omega_D$ will be assumed large compared with $[\Gamma_{ab}^2 + 2\Gamma_{ab} W \times (\Gamma_{aa}^{-1} + \Gamma_{bb}^{-1})/\pi]^{1/2}$. We have

$$-P''(\omega) = \int \frac{dv\,W(\omega)\Gamma_{ab}\hbar\,\Delta\rho(v)\,g_D(v)/\pi}{[\omega - \omega_{ba}(v)]^2 + \Gamma_{ab}^2 + (2\Gamma_{ab}\,W/\pi)[(1/\Gamma_{aa}) + (1/\Gamma_{bb})]} \simeq \frac{W(\omega)\Gamma_{ab}\hbar\,\Delta\rho g_D(\omega - \omega_{ba})}{\{\Gamma_{ab}^2 + 2\Gamma_{ab}\,W[(1/\Gamma_{aa}) + (1/\Gamma_{bb})]\pi^{-1}\}^{1/2}}\,, \quad (13)$$

where

$$W = \int_0^\infty W(\omega)\,d\omega$$

is the frequency-integrated rate of transition ($\sec^{-2}$) and

$$g_D(\omega - \omega_{ba}) = [\delta\omega_D\sqrt{\pi}\,]^{-1}\exp[-(\omega - \omega_{ba})^2/\delta\omega_D^2]$$

is the corresponding Doppler line shape in frequency rather than in velocity.

E. Inhomogeneous Broadening, Broadband Signal, and Moderate Saturation

By similar reasoning, upon using Eq. (11), we obtain

$$-P''(\omega) \simeq \int \frac{W(\omega)[\Gamma_{ab} + W(\omega)]\,\hbar\,\Delta\rho_{sat}(v)\,g_D(v)\,dv/\pi}{[\omega - \tilde{\omega}_{ba}(v)]^2 + [\Gamma_{ab} + W(\omega)]^2}\,,$$

where the population inversion at velocity v is

$$\Delta\rho_{sat}(v) = \Delta\rho\,[1 + K_{ab}(0)G]^{-1},$$

$$\tilde{\omega}_{ba}(v) = \omega_{ba}(1 + v/c) - \Omega(\omega)\,,$$

and

$$G = \int \frac{W(\omega)[\Gamma_{ab} + W(\omega)]\,d\omega/\pi}{[\omega - \tilde{\omega}_{ba}(v)]^2 + [\Gamma_{ab} + W(\omega)]^2} \simeq W(\omega_{ba}(v))\,,$$

when $\Gamma_{ab} + W(\omega_{ba}) \ll \delta\omega$, the spectral half-width of $W(\omega)$. Then, the integral over v, for large $\delta\omega_D$ and $\delta\omega$, yields the following power spectrum:

$$-\omega P''(\omega) \simeq \frac{W(\omega)\,\hbar\omega\Delta\rho g_D(\omega - \omega_{ba})}{1 + (\Gamma_{aa}^{-1} + \Gamma_{bb}^{-1})\,W(\omega)}\,, \quad (14)$$

since the integrand is sharply peaked at $\omega_{ba}(v) = \omega$, upon neglecting $\Omega(\omega)$.

F. Inhomogeneous Broadening, Broadband Signal, and Extreme Saturation

When the transition rate $W(\omega)$ for $|\omega - \omega_{ba}| \lesssim \delta\omega$ is much larger than $\delta\omega$ [the half-width of $W(\omega)$ itself], we have from the expressions just preceding Eq. (12)

$$\Delta\rho_{sat}(v) \simeq \Delta\rho\left[1 + \left(\frac{1}{\Gamma_{aa}} + \frac{1}{\Gamma_{bb}}\right) \times \int_0^\infty \frac{W(\omega)\,d\omega\,\Gamma_{ab}/\pi}{[\omega - \omega_{ba}(v)]^2 + \Gamma_{ab}^2 + 2\Gamma_{ab}\,W(\omega)}\right]^{-1}$$

$$\simeq \Delta\rho\left[1 + \left(\frac{1}{\Gamma_{aa}} + \frac{1}{\Gamma_{bb}}\right) \times \frac{W\Gamma_{ab}/\pi}{[\omega_0 - \omega_{ba}(v)]^2 + \Gamma_{ab}^2 + 2\Gamma_{ab}\,W(\omega_0)}\right]^{-1},$$

where we have assumed that $W(\omega)$ is peaked at $\omega = \omega_0$, not necessarily the line-center frequency. After the integration over v, and assuming $\delta\omega_D \ll \delta\omega$, we obtain Eq. (12) again. For

$$\delta\omega_D \gg [\Gamma_{ab}^2 + 2W(\omega_{ba})\Gamma_{ab}]^{1/2} \gg \delta\omega\,,$$

we obtain

$$-\omega P''(\omega) \simeq \frac{W(\omega)\Gamma_{ab}\,\hbar\,\omega\Delta\rho g_D(\omega_0 - \omega_{ba})}{[\Gamma_{ab}^2 + 2\Gamma_{ab}\,W(\omega_0) + (\Gamma_{aa}^{-1} + \Gamma_{bb}^{-1})\,W\Gamma_{ab}/\pi]^{1/2}}\,. \quad (15)$$

III. COMPARISON WITH PREVIOUS WORK

As already mentioned, the spectral power distribution for the quasimonochromatic case A agrees with the results for the true monochromatic case (as given by Javan[6] when all damping constants equal τ^{-1} and by Heer and Settles[1]) except for a doubling of the term proportional to the intensity in the linewidth squared. This doubling has been correctly described by Bender[2] in his perturbation analysis as due to the amplitude fluctuations that are not present in the true monochromatic case. However, in evaluating the saturation in this weak-signal approximation, Bender has incorrectly integrated the equations of motion for his second-order density-matrix elements found at the top of p. 563 of Ref. 2; thus the coefficient for self-saturation I_1 should be given by

$$I_1 = 2\,\mathrm{Re}\int_{-\Delta}^{\Delta}\int_{-\Delta}^{\Delta}(\Gamma+ix)^{-1}\left[\left(\frac{1}{\Gamma+ix}+\frac{1}{\Gamma-iy}\right)\times\frac{\Gamma}{\Gamma+i(x-y)}+\frac{1}{\Gamma+iy}+\frac{1}{\Gamma-iy}\right]dx\,dy\ ,$$

$$I_2 = 2\int_{-\Delta}^{\Delta}\frac{\Gamma dx}{\Gamma^2+x^2}\int_{-\Delta}^{\Delta}\frac{\Gamma dy}{\Gamma^2+y^2} = 2\pi^2\ ,$$

where I_2 is the coefficient for cross saturation by a signal of opposite circular polarization connecting level a with another level c which has similar properties to that of b. For simplicity, the signal was assumed by Bender to be uniform in intensity over a bandwidth Δ, and the levels were assumed to have the same damping factor Γ. For $\Delta \gg \Gamma$ (the broadband case B) we have $I_1 \simeq 2I_2 + O(\Gamma/\Delta)$, where $O(\Gamma/\Delta)$ denotes the negligible contribution of the term in I_1 that contains $[\Gamma+i(x-y)]^{-1}$. For the quasimonochromatic case, this term contributes equally to the others making $I_1 \simeq 4I_2$, as reported by Bender. When corrected and trivially reinterpreted, Bender's analysis would agree with the spectral power distribution that we obtained in case B above if we expand our result in powers of $2W(\omega)\Gamma_{ab}[(\omega-\omega_{ba})^2 + \Gamma_{ab}^2]^{-1}$ and then compare the resulting first-order term with the integrand in Bender's self-saturation term in $\langle R_+^{(4)}\rangle$, the stimulated emission rate that he calculated up to fourth order in the electric field. The result obtained by us for the broadband case E, dealing with an inhomogeneously broadened resonance and moderate saturation rate, disagrees with that of Heer with regard to line shape and to population saturation. In order to compare quantities similar to Heer's, we obtain the saturated gain coefficient $\beta(\omega)$ (cm^{-1}) from the quantity $-\omega P''(\omega)$ in Eq. (14) by dividing it by the intensity, that is,

$$\beta(\omega) = -8\pi\omega P''(\omega)/F(\omega)c \simeq \beta_0(\omega)\,[1+(\Gamma_{aa}^{-1}+\Gamma_{bb}^{-1})\,W(\omega)]^{-1}\ , \qquad (16)$$

where

$$\beta_0(\omega) = (2\pi)^2\,|\mu_{ab}|^2\Delta\rho\omega g_D(\omega-\omega_{ba})(\hbar c)^{-1}$$

is the unsaturated gain coefficient. This expression clearly reduces to the well-known unsaturated inhomogeneously broadened gain coefficient when $W(\omega)$ terms are neglected in Eq. (16). However, Heer's expression for $\beta(\omega)$, given in our notation and obtained from his Eq. (34) after integrating over the Doppler distribution for inhomogeneous broadening, differs from Eq. (16) by having $W(\omega)$ divided by 2π. The saturation of the population inversion when a broadband signal is present removes population at a rate $W(\omega)$, not $W(\omega)/2\pi$, compared to the rates Γ_{aa} and Γ_{bb}. Indeed, Eq. (16) is easily obtained from the rate equations for the steady-state populations. However, rate equations are applicable only when the line broadening effect of the rate $W(\omega)$ on a given molecule can be neglected. Heer's Eq. (34) neglects line broadening by $W(\omega)$, but our corresponding Eq. (11) does not.

The line broadening terms are not negligible and may be identified with Raman-type *self*-saturation terms having the factor $\Gamma[\Gamma+i(x-y)]^{-1}$ in our corrected form of Bender's coefficient I_1. For moderate saturation, we have found that these terms, however, contribute to the *integrated* power output only to order (Γ/Δ) compared to the dominant terms for weak signals of bandwidth Δ, in agreement with Bender. However, when the transition rate $W(\omega)$ becomes comparable to its own bandwidth, then these Raman-type terms become significant even in the integrated power output, the results resembling that for the quasimonochromatic case.

IV. STEADY TRAVELLING-WAVE BROADBAND MASER AMPLIFIER

The increase of maser intensity $I(x, \omega)$ with distance x, assuming propagation only along this direction, will now be equated to the power generated at frequency ω for the case E. Or, in terms of the gain coefficient $\beta(x, \omega)$ Eq. (16), the x dependence being now included, we have

$$\frac{dI(x,\omega)}{dx} = \beta(x,\omega)I(x,\omega)+\gamma(x,\omega)\ , \qquad (17)$$

where $\gamma(x, \omega)$ is the power generated per unit volume due to spontaneous emission, a process which we will not include hereafter. The amplifier will be considered to act on a weak input intensity $I_0(\omega)$ at $x=0$. The results will not differ substantially whether $I_0(\omega)$ has a very flat spectrum or a width equal to the Doppler width, that is, the width of $\beta(0, \omega)$. The inclusion of spontaneous emission $\gamma(x, \omega)$ will likewise not appreciably alter the results, and furthermore it is usually a weak source, of width comparable to that of $\beta(x, \omega)$, for the cosmic masers. Figure 1 shows the intensity calculated from Eqs. (16) and (17) as a function of frequency, measured from line center and in units of the Doppler half-width $\delta\omega_D$ at e^{-1} of maximum. Each curve corresponds to a value of αx, where α equals the line-center value of the unsaturated gain coefficient $\beta_0(\omega)$. Note the narrowing and then the broadening of the line as saturation sets in.

The line narrowing by a factor of approximately $(\alpha x)^{-1/2}$ of a broadband signal due to travelling-wave amplification over a length x is well known, but the behavior of the linewidth after saturation occurs is rarely discussed. If the intensity $I(x, \omega)$ at some position x along the propagation path and at some frequency ω (measured relative to the line-center frequency ω_{ba}) is parametrized by a nearly Gaussian shape, with amplitude and bandwidth which are functions of x alone, then we have

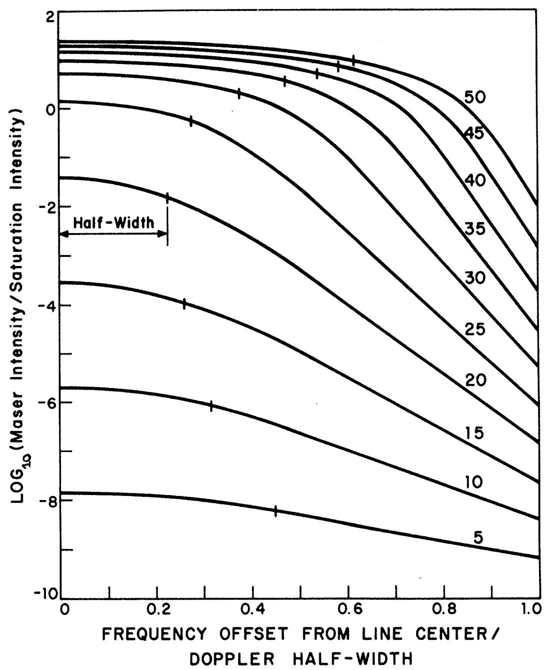

FIG. 1. Logarithm of the output maser intensity (divided by the saturation parameter I_s) as a function of frequency (measured from resonance line center and in units of the Doppler half-width at e^{-1} of maximum) for ten different distances along the amplifier (multiplied by the unsaturated gain coefficient at line center). The input intensity I_0 equals 10^{-10} I_s. The input spectrum is flat. The half-widths at e^{-1} of maximum are marked for the calculated intensities.

$$I(x, \omega) \simeq I(x) e^{-\omega^2/\Delta\omega(x)^2} .$$

The emission rate, obtained from Eq. (14), is set equal to the increase of intensity with distance:

$$\frac{dI(x, \omega)}{\alpha dx} \simeq \frac{I(x, \omega) e^{-\omega^2/\delta\omega_D^2}}{1 + I(x, \omega)/I_s} . \tag{18}$$

Equation (18) is integrated to yield

$$\ln\{[I(x)/I_0] e^{-\omega^2/\Delta\omega^2}\} + [I(x)/I_s] e^{-\omega^2/\Delta\omega^2} - I_0/I_s$$
$$\simeq \alpha x e^{-\omega^2/\delta\omega_D^2} .$$

The boundary condition at $x = 0$ that $I = I_0$ and $\Delta\omega = \infty$, i.e., that there is a broad continuum at the input, has been incorporated in the above solution. In the saturated case, with large amplification ($I_s \gg I_0$), we have

$$\frac{I(x)}{I_s} e^{-\omega^2/\Delta\omega^2} + \ln\frac{I(x)}{I_s} \simeq \alpha x e^{-\omega^2/\delta\omega_D^2} + \frac{\omega^2}{\Delta\omega^2} - \alpha x_s + 1 ,$$

where $x_s = (1/\alpha) [\ln(I_s/I_0) + 1]$ is the distance at which nearly exponential growth (the second term of unity being due to saturation) would bring the intensity up to the value I_s. The last three terms arise from the approximate expression for $I(x, \omega)$ in the "ln" term. Upon equating the leading terms in the power series expansion in ω^2, we obtain

$$I(x)/I_s \simeq \alpha(x - x_s) + 1 - \ln[1 + \alpha(x - x_s)] \quad \text{for } x \geq x_s \tag{19}$$

and

$$\frac{(I/I_s) + 1}{\Delta\omega^2} \simeq \frac{\alpha x}{\delta\omega_D^2} .$$

Therefore, we have

$$\Delta\omega/\delta\omega_D \simeq \{\alpha(x - x_s) - \ln[1 + \alpha(x - x_s)] + 2\}^{1/2}$$
$$\times [\alpha x]^{-1/2} \to 1 \text{ as } x \to \infty . \tag{20}$$

Therefore, the bandwidth which was narrowed by $(\alpha x_s/2)^{-1/2}$, the extra factor of $\sqrt{2}$ being due to saturation effects up to $x = x_s$, is then broadened in saturated growth by the factor

$$\{\alpha(x - x_s) - \ln[1 + \alpha(x - x_s)] + 2\}^{1/2}(2x/x_s)^{-1/2} \text{ for } x > x_s .$$

x_s is the distance at which saturation is becoming dominant. Eventually, the width approaches the Doppler width. For example, if $\alpha x_s \simeq 24$, for amplification by 10^{10} at x_s, then at $x = 2x_s$ the linewidth is that at x_s, namely, $\delta\omega_D/(12)^{1/2}$, but then multiplied by a factor of 2.4 due to the wave propagation from x_s to $2x_s$, resulting in a linewidth $\delta\omega \simeq 0.7\delta\omega_D$, which is about 15% higher than obtained in Fig. 1.

Finally, we compare these results with the perturbation analysis given by Parks,[7] who has derived an approximate radiative transport equation like Eq. (18) from the polarization $\vec{\mathcal{P}}(\omega)$, Eq. (4), calculated only to third order in electric fields. His equation, given in our notation where appropriate, is

$$\frac{dI(x, \omega)}{dx}$$
$$= \alpha I(x, \omega) \left(e^{-\omega^2/\delta\omega_D^2} - \frac{S}{I_0} \int_0^\infty d\omega' I(x, \omega') A_{\omega\omega'} \right) ,$$

where the kernel $A_{\omega\omega'}$ involves an integral over the velocity distribution, $I_0(\omega)$ is the incident spectral intensity having a bandwidth equal to the Doppler width. The saturation parameter is $S = 8\pi |\mu_{ab}|^2 \times I_0 \sqrt{\pi}\, \delta\omega_D (2\hbar^2 c \Gamma_{aa} \Gamma_{bb})^{-1}$, while the saturation intensity I_s in Eq. (18) is found to be

$$I_s = [4\pi^2 |\mu_{ab}|^2 (\Gamma_{aa}^{-1} + \Gamma_{bb}^{-1})/(\hbar^2 c)]^{-1}$$

upon comparing Eqs. (16) and (18). The kernel

$$A_{\omega\omega'} \simeq 2\sqrt{\pi}\, (\Gamma_{ab}/\delta\omega_D) e^{-\omega^2/\delta\omega_D^2} \delta(\omega - \omega')$$

when $\Gamma_{ab} \ll \delta\omega_D$, as assumed in Eqs. (14), (16), and (18). We now see that the Parks equation is just Eq. (18) with $[1 + I(x, \omega)/I_s]^{-1}$ approximated by $1 - I(x, \omega)I_s$. The linewidth calculated by Parks when

$S=5\times10^{-3}$ and $\Gamma_{ab}=10^{-2}\,\delta\omega_D$ for $\alpha x<12$ is slightly larger than our calculated linewidths for the corresponding parameters:

$$\frac{I_s}{I_0}=\left(2\sqrt{\pi}\,\frac{S\Gamma_{ab}}{\delta\omega_D}\right)^{-1}=\frac{10^4}{\sqrt{\pi}}\quad\text{and } \alpha x_s\simeq 8.8\ .$$

According to an extension of the analysis leading to Eqs. (19) and (20) so that $\Delta\omega$ at $x=0$ is $\delta\omega_D$ instead of infinity, we merely replace αx by $\alpha x+1$ in the denominator of the expression (20) for $\Delta\omega/\delta\omega_D$. Equation (20) so modified gives for $x=x_s$, $\Delta\omega/\delta\omega_D\simeq 0.45$, the same as Parks's result.

We mention that the signal bandwidth for the inhomogeneously broadened case C has also been found, similarly to Eq. (20), to be

$$\Delta\omega\simeq\frac{[\Gamma_{ab}^2+2\Gamma_{ab}W(0)]^{1/2}}{[\ln I(x)/I_0]^{1/2}}\quad ,$$

where $W(0)$ is the transition rate at line center induced by the intensity $I(x)$, a complicated monotonic function of the amplification distance. The rapid broadening implied here occurs only when $\Delta\omega\gg\Gamma_{ab}$. However, when $\Delta\omega\lesssim\Gamma_{ab}$, slower broadening with increasing x is expected, a different conclusion than reached by Icsevgi and Lamb.[8]

V. CONCLUDING REMARKS

The spectral power distribution as presented here has limited application mainly because of the use of Gaussian statistics. While examination of the OH maser data so far has justified this assumption, numerous examples of amplifiers of coherent pulses exist in the laboratory. Another limitation concerns our lack of a description of the transition region as a function of intensity between the case of moderate saturation and that of extreme saturation, although this could be obtained from a solution of the integral equation (8). From estimates of the saturation rate $W(\omega)<10\ \text{sec}^{-1}$ for the OH and H_2O masers and the known signal bandwidths $\delta\omega\simeq10^4$–$10^5\ \text{sec}^{-1}$, we think it probable that the transition to extreme saturation when $W(\omega)\gtrsim\delta\omega$ need not arise.[4]

Time variations observed over weeks in the H_2O emission have suggested that the amplifier is not saturated, while the usually steady OH emission over months or years would strongly suggest saturation. The narrow OH lines then imply that the kinetic temperatures are low, sometimes less than 10 °K, rather than that unsaturated maser narrowing has occurred at hundreds of degrees. Cross-relaxation processes within the molecular velocity distribution have not been included in our analysis. These would prevent line broadening despite population saturation if the cross-relaxation rate exceeds $W(\omega)$, but Γ_{aa} or Γ_{bb} do not.[3] Collisions by hydrogen atoms or molecules are the most likely means of sufficiently fast cross relaxation, but then Γ_{aa} and Γ_{bb} would also be large owing to such collisions – too large for saturation to occur. The behavior of the bandwidth with distance for cases for which the signal bandwidth is comparable to the homogeneous linewidth will be dealt with in a future paper.

Finally, the neglect of spontaneous emission is perhaps justified for the interstellar masers, considering that the interferometer sizes of the several emitting points in a given region appear to be much smaller than the amplifier sizes implied by the time variations. This implies that we are observing images of "hot spots" or apparent sources in a large amplifier. For the OH near H II regions, the signal is usually highly circularly polarized, an effect believed to be caused by saturation and nonlinear competition between oppositely polarized modes.[4] If spontaneous emission were important compared to the hot-spot emission, the interferometer sizes would be comparable to that of the amplifier. The spontaneous emission may not compete well for saturating the amplifier, not only because of low (negative) excitation temperatures, but also because radial flow velocities would restrict the solid angles over which spontaneous emission coming from remote regions would be resonant with molecules at a given point in the amplifier. Perhaps filamentary structure to the amplifier is also implied. In the output intensity and linewidth derived in Sec. IV, we assumed that the saturation parameter I_s was independent of distance along the amplifier. This appears reasonable since the solid angle over which there is appreciable maser intensity (at any point in the amplifier) and also the damping constants may be decreasing with the square of the distance along the amplifier, that is, the distance from the apparent microwave source. The radiative transport equation (17) then is trivially reinterpreted to apply to the brightness, the intensity per *steradian*. But I_s involves the brightness integrated over the local solid angle to determine the total saturation rate acting on a molecule divided by an effective damping rate. This rate is probably determined either by optical pumping that decreases with the square of the distance from the pump sources, which we assume lie in the vicinity of or perhaps coincide with the apparent microwave sources, or by collisions, with a rate that decreases similarly because the density is likely to decrease nearly as the square of the distance from condensed objects such as these.[4,9]

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Unique Definition of the Quasistationary State for Resonant Processes

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The quasistationary-state formalism for describing all manner of resonant collision processes and the diabatic states of molecules is made unique by defining the hitherto arbitrary quasistationary-state energy uniquely. The unique quasistationary-state energy E_r (together with its wave function) is defined by a pair of eigenvalue equations which require that it remain unshifted by coupling to the continuum. Two alternate and equivalent definitions are also given, and the results are generalized first to the many-resonance case and secondly in the unusual direction of negative energies, where the quasistationary state produces a resonance among the discrete set of Rydberg levels. This last generalization is necessary for the principal present application of the states, i.e., to the diabatic states mediating molecular transitions, since the energy of these diabatic states moves freely between the continuum and the negative-energy region of the Rydberg states.

I. INTRODUCTION

For the mathematical description of either resonant elastic and inelastic scattering[1] or of rearrangement and other diatomic collision processes proceeding through a resonant state,[2,3] probably the most simple, elegant, and practical approach is the quasistationary-state formalism whose essential points trace back to Dirac.[4]

In the quasistationary-state formalism, one first defines a bounded wave function χ_r which should be some approximation to the close-in part of the scattering wave function at resonance and which defines the quasistationary-state energy ϵ_r. The full wave function and Hamiltonian are then partitioned by the use of a projection operator onto this function, and the Schrödinger equation is formally solved in such a way as to exhibit the dependence on the resonance parameters most explicitly.

The quasistationary-state function χ_r upon which the formalism hinges is mathematically quite arbitrary, thus making its energy ϵ_r arbitrary, a fact which is both a strength and a weakness. Its strength lies in the flexibility it allows to anyone doing a fully *ab initio* theoretical calculation, a flexibility which is widely exploited in a variety of calculational methods.[5] Its weakness, which is more of a conceptual than a practical one, shows up either in semiempirical analyses of experiments (which seem to be the most fruitful way of exploiting the theory) or in very general or formal descriptions of what is happening. In either case, one really would like not just an arbitrary quasistationary-state energy but a unique state, a point which has been well made by Smith.[6] The fact that the final answers in the quasistationary-state formalism are unique in any application, thanks to a compensating level shift Δ, is not satisfying enough from a conceptual point of view, and a need for a unique definition of the quasistationary-state energy is seriously felt. To fill this need is the purpose of the present paper.

Section II briefly reviews the quasistationary-state formalism description of resonant elastic or inelastic scattering, in order to introduce and define the necessary concepts. The unique definition of the quasistationary state is presented in Sec. III and then restated in two equivalent ways. In Sec. IV the many-resonance generalizations of Secs. II and III are given. Section V generalizes the result in a different direction, to quasistationary states whose energy lies not in the continuum but at negative energy, among a discrete set of Rydberg energy levels. This is necessary for any application