Quantum 1/f and Classical Phase Noise in Resonant Bio-Chemical MEMS Sensors

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Abstract: *While classical physics provides no universal 1/f spectrum, quantum mechanics and electrodynamics require the presence of fundamental quantum fluctuations of physical currents, cross sections, and process rates, because of the infrared quasi-divergence and radiative corrections. The present paper calculates these quantum fluctuations, shows that they have a simple universal 1/f spectrum, and shows how they invariably come to the foreground, being dominant at low frequencies in high-technology applications. This happens because in them all other fluctuations and sources of instability have been either eliminated, or otherwise discounted and put under control. BAW, SAW and MEMS resonators are no exception. This defines detection limits and optimization rules for biological and chemical sensors based on them.*

I. INTRODUCTION

It is well known that fluctuations with a spectral density proportional to 1/f are found in a large number of systems in science, technology and everyday life. These fluctuations are known as 1/f noise in general. They have first been noticed by Johnson [1] in early amplifiers, have limited the performance of vacuum tubes in the thirties and forties, and have later hampered the introduction of semiconductor devices and nano-devices.

1/f noise is present as a limitation in most modern high-technology devices. It is present in the resonance frequency of bulk acoustic wave (BAW) quartz resonators, in surface acoustic wave (SAW) devices, in junction and MIS infrared detectors, in superconducting quantum interference devices (SQUIDs), in electron beams, micro-electro-mechanical systems (MEMS), etc. Outside the domain of electrophysics 1/f noise is present in a wide variety of circumstances and systems. It was found in the rate of radioactive decay, in the flow rate of sand in an hourglass, in the flux of cars on an expressway, in the frequency of sunspots, in the light output of quasars, in the flow rate of the Nile over the last 2,000 years, in the water current velocity fluctuations at a depth of 3,100 meters in the Pacific ocean, and in the loudness and pitch fluctuations of classical music. It has also been found below 10^{-8} Hz in the angular velocity of the earth's rotation, and below 10^{-4} Hz in the relativistic neutron flux in the terrestrial atmosphere [2].

The present paper is focused on fundamental 1/f noise and phase noise. It starts in sec. II with a special case of the general 1/f noise phenomenon, the Quantum 1/f Effect which is a new aspect of quantum mechanics. This is applied to quartz resonators in Sec. III and to MEMS resonators in Sec. IV. In addition, classical sources of frequency and phase fluctuations are reviewed in Sec. V. Illustrative numerical estimates are shown in Sec. VI. Applications to sensors are in Sec. VII.

II. CONVENTIONAL QUANTUM 1/F EFFECT

This effect [3-18] is present in any cross section or process rate involving charged particles or current carriers. The physical origin of quantum 1/f noise is easy to understand. Consider for example Coulomb scattering of current carriers, e.g., electrons on a center of force. The scattered electrons reaching a detector at a given angle away from the direction of the incident beam are described by DeBroglie waves of a frequency corresponding to their energy. However, some of the electrons have lost energy in the scattering process, due to the emission of bremsstrahlung. Therefore, part of the outgoing DeBroglie waves is shifted to slightly lower frequencies. When we calculate the probability density in the scattered beam, we obtain also cross terms, linear both in the part scattered with and without bremsstrahlung. These cross terms oscillate with the same frequency as the frequency of the emitted bremsstrahlung photons. The emission of photons at all frequencies results therefore in probability density fluctuations at all frequencies. The corresponding current density fluctuations are obtained by multiplying the probability density fluctuations by the velocity of the scattered current carriers. Finally, these current fluctuations present in the scattered beam will be noticed at the detector as low frequency current fluctuations, and will be interpreted as fundamental cross section fluctuations in the scattering cross section of the scatterer. While incoming carriers may have been Poisson distributed, the scattered beam will exhibit super-Poissonian statistics, or bunching, due to this new effect which we may call quantum 1/f effect. The quantum 1/f effect is thus a many-body or collective effect, at least a two-particle effect, best described through the two-particle wave function and two-particle correlation function.

Let us estimate the magnitude of the quantum 1/f effect semiclassically. We start with the classical (Larmor) formula $2q^2\mathbf{a}^2/3c^3$, for the power radiated by a particle of charge q and acceleration **a**. The acceleration can be approximated by a delta function $\mathbf{a}(t) = \Delta\mathbf{v}\delta(t)$ whose Fourier transform $\Delta\mathbf{v}$ is constant and is the change in the velocity vector of the particle during the almost instantaneous scattering process. The one-sided spectral density of the emitted bremsstrahlung power $4q^2(\Delta \mathbf{v})^2/3c^3$ is therefore also constant. The number $4q^2(\Delta \mathbf{v})^2/3hfc^3$ of emitted photons per unit frequency interval is obtained by dividing with the energy hf of one photon. The probability amplitude of photon emission $[4q(\Delta \mathbf{v})^2/3hfc^3]^{1/2}e^{i\gamma}$ is given by the square root of this photon number spectrum, including also a phase factor $e^{i\gamma}$. Let ψ be a representative Schrödinger catalogue wave function of the scattered outgoing charged particles, which is a single-particle function, normalized to the actual scattered particle concentration. The beat term in the probability density $\rho=|\psi|^2$ is linear both in this bremsstrahlung amplitude and in the non-bremsstrahlung amplitude. Its spectral density will therefore be given by the product of the squared probability amplitude of photon emission (proportional to 1/f) with the squared non-bremsstrahlung amplitude which is independent of f. The resulting spectral density of fractional probability density fluctuations is obtained by dividing with $|\psi|^4$ and is therefore

$$|\psi|^{-4}S_{|\psi|^2}(f) = 8q^2(\Delta \mathbf{v})^2/3hfNc^3 = 2aA/fN = j^{-2}S_j(f), \qquad (2.1)$$

where $\alpha = e^2/\hbar c = 1/137$ is the fine structure constant and $\alpha A = 4q^2(\Delta \mathbf{v})^2/3hc^3$ is known as the infrared exponent in quantum field theory, and is known as the quantum 1/f noise coefficient, in electrophysics. The experimentally measured quantity also depends on many superposition or averaging processes and is often called, for historical reasons, Hooge constant.

The spectral density of current density fluctuations is obtained by multiplying the probability density fluctuation spectrum with the squared velocity of the outgoing particles. When we calculate the spectral density of fractional fluctuations in the scattered current j, the outgoing velocity simplifies, and therefore Eq. (2.1) also gives the spectrum of current fluctuations $S_j(f)$, as indicated above. The quantum 1/f noise contribution of each carrier is independent, and therefore the quantum 1/f noise from N carriers is N times larger. However, the current j will also be N times larger, and therefore in Eq. (2.1) a factor N was included in the denominator, for the case in which the cross section fluctuation is observed on N carriers simultaneously.

The fundamental fluctuations of cross sections and process rates are reflected in various kinetic coefficients in condensed matter, such as the mobility μ and the diffusion constant D, the surface and bulk recombination speeds s, and recombination times τ, the rate of tunneling j_t and the thermal diffusivity in semiconductors. Therefore, the spectral density of fractional fluctuations in all these coefficients is given also by Eq. (2.1).

When we apply Eq. (2.1) to a certain device, we first need to find out which are the cross sections σ or process rates that limit the current I through the device, or that determine any other device parameter P. Then we have to determine both the velocity change $\Delta \mathbf{v}$ of the scattered carriers and the number N of carriers simultaneously used to test each of these cross sections or rates. Further, Eq. (2.4) provides the spectral density of quantum 1/f cross section or rate fluctuations. These spectral densities are multiplied by the squared partial derivative $(\partial I/\partial \sigma)^2$ of the current, or of the device parameter P of interest, to obtain the spectral density of fractional device noise contributions from the cross sections and rates considered. After doing this with all cross sections and process rates, we add the results and bring (factor out) the fine structure constant α as a common factor in front. This yields excellent agreement with the experiment [7-9], in a large variety of samples, devices and physical systems.

Eq. (2.4) was also derived in second quantization [6], [12], [15], [17], using the commutation rules for boson field operators. For fermions one repeats the calculation replacing in the derivation the commutators of field operators by anticommutators, which yields

$$\rho^{-2}S_\rho(f) = j^{-2}S_j(f) = \sigma^{-2}S_\sigma(f) = 2\alpha A/f(N-1). \qquad (2.2)$$

This causes no difficulties, since $N \geq 2$ for particle correlations to be defined, and is practically the same as Eq. (2.1), since usually N>>1. Eqs. (2.1) and (2.2) suggest a new notion of physical cross sections and process rates which contain 1/f noise, and express a fundamental law of physics, important in most high-technology applications.

III. Quantum 1/f Effect in Frequency Standards

Frequency standards contain a main resonant mode which can be described as a harmonic oscillator with losses

$$dx/dt + \gamma dx/dt + \omega_o^2 x = F(t). \qquad (3.1)$$

The quantum 1/f fluctuations are present in the loss coefficient γ. They are given by an expression of the form

$$S_{\delta\gamma/\gamma}(f) = \Lambda/f, \qquad (3.2)$$

where Λ is a quantum 1/f coefficient characterizing the elementary loss process. The resonance frequency is given by

$$\omega_r^2 = \omega_o^2 + \gamma^2. \qquad (3.3)$$

The quantum 1/f fluctuations in the resonance frequency are given by $\omega_r\delta\omega_r = -2\gamma\delta\gamma$, or

$$\delta\omega_r/\omega_r = -2(\gamma/\omega_r)^2\delta\gamma/\gamma = -(1/2Q^2)(\delta\gamma/\gamma), \qquad (3.4)$$

where $Q=\omega_r/2\gamma$ is the quality factor. Squaring, averaging and particularizing Eq. (3.4) for the unit frequency interval, we obtain the Q^{-4} law [18]

$$S_y(f) = \langle(\delta\omega_r/\omega_r)^2\rangle_f = (1/4Q^4)\langle(\delta\gamma/\gamma)^2\rangle_f = \Lambda/4fQ^4, \qquad (3.5)$$

where y is the fractional frequency fluctuation $\delta\omega_r/\omega_r$. This law was found in approximative form empirically by Gagnepain and Uebersfeld for the case of quartz resonators. The coefficient Λ is calculated for an ideal quartz crystal as follows.

According to the general quantum 1/f formula in Eq. (2.1), $\Gamma^{-2}S_\Gamma(f)=2\alpha A/f$, where $A=2(\Delta \mathbf{J}/ec)^2/3\pi$ is the quantum 1/f effect in any physical process rate Γ. Setting $\mathbf{J}=d\mathbf{P}/dt=\dot{\mathbf{P}}$ where $\mathbf{P}$ is the vector of the dipole moment of the quartz crystal, we obtain for the fluctuations in the rate Γ of phonon removal from the main resonator oscillation mode (by scattering on a phonon from any other mode of average frequency $\langle\omega\rangle$) of the crystal, (or via a two-phonon-process at a crystal defect or impurity, involving a phonon of average frequency $\langle\omega'\rangle$) the spectral density

$$S_\Gamma(f) = \Gamma^2 4\alpha(\Delta\dot{\mathbf{P}})^2/3\pi e^2c^2, \qquad (3.6)$$

where $(\Delta\dot{\mathbf{P}})^2$ is the square of the dipole moment rate change associated with the process causing the removal of a phonon from the main oscillator mode. To calculate it, we write the energy W of the interacting resonator mode $\langle\omega\rangle$ in the form

$$W = n\hbar\langle\omega\rangle = 2(Nm/2)(dx/dt)^2$$
$$=(Nm/e^2)(e\,dx/dt)^2=(m/Ne^2)\varepsilon^2(\dot{\mathbf{P}})^2; \qquad (3.7)$$

The factor two includes the potential energy contribution. Here m is the reduced mass of the elementary oscillating dipoles, e their charge, ε a polarization costant, and N their number in the quartz crystal. Applying a variation $\Delta n=1$ we get

$$\Delta n/n = 2|\Delta\dot{\mathbf{P}}|/|\dot{\mathbf{P}}|, \text{ or } \Delta\dot{\mathbf{P}} = \dot{\mathbf{P}}/2n. \qquad (3.8)$$

Solving Eq. (3.7) for $\dot{\mathbf{P}}$ and substituting, we obtain

$$|\Delta\dot{\mathbf{P}}| = (N\hbar <\omega>/n)^{1/2}(e/2\varepsilon) \qquad (3.9)$$

Substituting $\Delta\dot{\mathbf{P}}$ into Eq. (3.6), we get

$$\Gamma^{-2}S_{\Gamma}(f) = N\alpha\hbar <\omega>/3n\pi mc^2 f\varepsilon^2 \equiv \Lambda/f\,. \qquad (3.10)$$

This result is applicable to the fluctuations in the loss rate Γ of the quartz. For other frequency standards see [24].

The corresponding resonance frequency fluctuations of the quartz resonator are given by

$$\omega^{-2}S_{\omega}(f) = (1/4Q^4)(\Lambda/f) = N\alpha\hbar <\omega>/12n\pi mc^2 f\varepsilon^2 Q^4, \quad (3.11)$$

where Q is the quality factor of the single-mode quartz resonator considered, and $<\omega>$ is not the circular frequency of the main resonator mode, ω_0, but rather the practically constant frequency of the average interacting phonon, considering both three-phonon and two-phonon processes. The corresponding $\Delta\dot{\mathbf{P}}$ in the main resonator mode has to be also included in principle, but is negligible because of the very large number of phonons present in the main resonator mode.

Eq. (3.11) can be written in the form

$$S(f) = \beta V/fQ^4, \qquad (3.12)$$

where, with an intermediary value $<\omega>=10^8$/s, with $n=kT/\hbar <\omega>$, T=300K and $kT=4\ 10^{14}$,

$$\beta = (N/V)\alpha\hbar <\omega>/12n\pi\varepsilon^2 mc^2$$
$$=10^{22}(1/137)(10^{-27}10^8)^2/12kT\pi 10^{-27}\ 9\ 10^{20} = 1. \quad (3.13)$$

The form of Eq. (3.11) shows that the level of 1/f frequency noise depends not only as Q^{-4} as previously proposed[18], but also on the volume of the active region[14]. Note that the phonon removal process creates the largest electromagnetic bremsstrahlung due to the change in the thermal phonon number at the frequency $<\omega>$ that is associated with the same process. The average/effective frequency of an interacting thermal phonon can be calculated from the matrix elements and the phonon spectra, and can be considerably larger than the value assumed here.

A. The Case of Defect Scattering: a two-phonon process.

At low temperatures, there are few thermal phonons. Preferentially, a phonon from the main resonator mode scatters on a defect in this case, and a phonon of comparable frequency emerges into another mode with much smaller phonon occupation number $n_{\omega}=kT/\hbar\omega$. In this case, in Eq. (3.10) for Γ, and Eq. (3.13) for β we have to replace $<\omega>$ by ω and $n_{<\omega>}$ with n_{ω}, which gives a β-value which is $(<\omega>/\omega)^2$ smaller, i.e. 10^4-10^6 times smaller.

B. General Case

Let Γ' be the rate of phonon removal through 3-phonon processes, and Γ" the corresponding rate through two-phonon processes, caused by defects, including the surface of the sample. With $\Gamma=\Gamma' + \Gamma''$, being the total phonon removal rate from the main oscillation mode, we obtain for the combined phonon and defect scattering case, in general,

$$\beta=\beta'[\Gamma'^2 + (\omega/<\omega>)^2\Gamma''^2]/\Gamma^2. \qquad (3.14)$$

Although the defect scattering term is small at room temperature, it may become dominant at low temperatures or in ultra-small crystals, when the phonon scattering rate Γ' becomes much smaller than the defect scattering rate Γ".

One obtains again Eq. (3.12), with β given by Eq. (3.14) in the final result, as shown in Fig. 1. Since the 1/f noise level depends on the active volume, in the coherent regime one should use the lowest overtone and smallest diameter consistent with other circuit parameters. In the incoherent (low Q) case, in which there are several independent domains in the quartz crystal, with statistically independent quantum 1/f fluctuation in their phonon removal rates, the opposite should be considered. This latter case is often observed in SAW devices.

IV. Silicon MEMS Resonator Sensors

The classical forms of noise present in the frequency of microelectromechanical systems (MEMS) resonators, have been recently investigated and described in detail [20], [21]. The present paper extends this investigation to 1/f noise. That is of fundamental nature in MEMS resonators, and is given by the universal quantum 1/f effect, with some similarities to the case of quartz resonators. When the environmental fluctuations are reduced, e.g., by temperature stabilization, elimination of molecular adsorption, etc., the fundamental limitation introduced by the quantum 1/f effect becomes visible as a flicker floor in the time-domain noise representation. Being ultimately based on Heisenberg's uncertainty relations, this effect defines the quantum limit achievable at low frequencies, when the classical sources of noise have been sufficiently reduced.

The quantum 1/f effect manifests itself in MEMS resonators through conventional quantum 1/f noise. This is a quantum fluctuation present in the quantum mechanical notion of "physical cross section" σ and "physical process rate" Γ, caused by the reaction of the electromagnetic field on the charged particle that emitted it, or in general, on the system that emitted it. It is given by the spectral density of fractional fluctuations, as in Eq. (2.1),

$$S_{\delta\sigma/\sigma}(f) = S_{\delta\Gamma/\Gamma}(f) = (4\alpha/3\pi f)(\Delta\mathbf{v}/c)^2, \quad (4.1)$$

where $\Delta\mathbf{v}$ is the velocity vector change of the current carriers of charge e. As shown in the case of BAW and SAW quartz resonators, or of ferroelectrics, the rate Γ of interest for the calculation of 1/f resonance frequency fluctuations in Si MEMS is the rate of phonon removal from the main mechanical oscillation mode of the oscillating bar, finger or cantilever. As in the above-mentioned cases, our mechanism of quantum 1/f noise generation is based on bremsstrahlung from electric or magnetic dipoles, rather than from scattering of individual carriers.

The MEMS resonators are shaped as a bar of micro- or nanometric dimensions, often incased (fixed) at both ends, and subject to bending strain. Sometimes they are free on both ends (that are antinodes in this case of "free-free" resonant bars), and are just supported at two nodal points. They are driven by an AC current I flowing in a very thin straight wire attached along the bar, in the presence of a strong constant magnetic field **B**, perpendicular to it. Most often, they are driven electrostatically, or capacitively, by using the wire, or a metallic thin sheet deposited along that side of the bar, as one of the two "plates" of a capacitor. An AC voltage would then be applied to the capacitor at the resonance frequency.

The approach developed above for the case of resonators based on quartz and other piezoelectric substances can not be applied to Si MEMS resonators, because silicon is not piezoelectric. It could only be applied to piezoelectric MEMS resonators, using, for instance, quartz. We therefore develop a new approach in this paper, applicable to the new, driven MEMS resonators. We consider below both the case of electrical and magnetic excitation.

A. Electrostatic Excitation of a Resonant Silicon Bar

The elementary act of dissipation is again the absorption of one phonon from the main resonator mode. This time, the quantum 1/f noise is caused by the sudden change in the rate of change of the dipole moment $\dot{\mathbf{p}}$ of the capacitor that excites the MEMS resonator bar, when the phonon is absorbed. Replacing the current change $e\Delta\mathbf{v}$ with $\Delta\dot{\mathbf{p}}$, we obtain

$$S_{\delta\Gamma/\Gamma}(f) = 4\alpha(\Delta\dot{\mathbf{p}})^2/3\pi f e^2c^2. \qquad (4.2)$$

To calculate the change $\Delta\dot{\mathbf{p}}$, we note that $(\dot{\mathbf{p}})^2$ is proportional to the squared transversal vibration speed of the bar and to the total mechanical energy $W=(n+1/2)\hbar\omega$ in the main oscillation mode of the resonator,

$$(n+1/2)\hbar\omega = \kappa'(\dot{\mathbf{p}})^2/2. \qquad (4.3)$$

Here κ' is a coefficient of proportionality easy to calculate. When a phonon is removed from the main MEMS resonator mode, the energy in Eq. (4.3) is reduced by the amount

$$\hbar\omega = \kappa'\dot{\mathbf{p}}\,\Delta\dot{\mathbf{p}}\,. \qquad (4.4)$$

This yields

$$(\Delta\dot{\mathbf{p}})^2 = (\hbar\omega/\kappa'\dot{\mathbf{p}})^2 = \hbar\omega/(2n+1)\kappa'. \qquad (4.6)$$

Eq. (4.2) becomes now

$$S_{\delta\Gamma/\Gamma}(f) = (4\alpha/3\pi f)\,\hbar\omega/(2n+1)\kappa'(ec)^2$$
$$=\underline{4\omega/3\pi f(2n+1)\kappa' c^3} = 2\hbar\omega^2/3\pi f W\kappa' c^3. \qquad (4.7)$$

This quantum 1/f noise, proportional to the resonance frequency and inversely proportional to the number of quanta in the main oscillation mode, decreases when the energy in the main resonator mode increases. This is characteristic of quantum mechanical spontaneous emission noise in general. With $\omega = 10^{12}$ rad/sec and $W=10^{-13}$ erg we obtain about $10^{-22}/f\kappa'$.

To estimate the coefficient κ', we write again the mechanical energy in the form

$$W = M_{eff}v^2/2. \qquad (4.8)$$

Noting that the rate of change in the electric dipole moment of the system, caused by the motion of the bar of linear charge density q is

$$\dot{\mathbf{p}} = qLv, \qquad (4.9)$$

we find

$$\kappa' = M_{eff}v^2/\dot{\mathbf{p}}^2 = M_{eff}/q^2L^2. \qquad (4.10)$$

With $M_{eff}=10^{-11}$g, $L=10^{-3}$cm and $q=0.6$ esu/cm, we obtain $\kappa'=2.7\cdot 10^{-5}s^2cm^{-3}$. Substituting into Eq. (4.7), we obtain

$$S_{\delta\Gamma/\Gamma}(f) = (4\alpha/3\pi f)q^2L^2\hbar\omega/(2n+1)M_{eff}(ec)^2$$
$$=\underline{4q^2L^2\omega/3\pi f(2n+1)M_{eff}c^3}$$
$$=2q^2L^2\hbar\omega^2/3\pi f W M_{eff}c^3. \qquad (4.11)$$

For instance, with the above numerical example, with $\omega=10^{12}s^{-1}$, and with $W=10^{-13}$ erg, we obtain $3\cdot 10^{-18}/f$.

B. Magnetic Excitation of a Resonant Silicon Bar

The elementary act of dissipation is the absorption of one phonon from the main resonator mode. This can happen either through three photon processes, dominant at higher temperatures, or through two processes, dominant at low temperatures, in the presence of crystal defects of various types. In both cases this elementary act has "bremsstrahlung photon emission (probability) amplitude" associated with it, because it causes a sudden reduction $\Delta\dot{\mathbf{m}}$ of the rate $d\mathbf{m}/dt \equiv \dot{\mathbf{m}}$ of change of the magnetic dipole moment vector **m** of the system. The system is defined here to include the current carrying circuit, the applied magnetic field **B** with the agency generating it, plus the oscillating bar, i.e., the MEMS. The rate $\dot{\mathbf{m}}$ of change of the magnetic dipole moment **m** of the system is caused by bending oscillations of the bar with the current-carrying wire attached to its side, cutting the lines of force of **B** while it moves. The vector $\mathbf{m} = \mathbf{n}SI/c$ is defined by the current I, enclosing the area S that has a normal of unit vector **n**.

The conventional quantum 1/f noise in the rate of dissipation Γ is obtained in the CGS Gaussian system by simply replacing the current change $e\Delta\mathbf{v}$ with $\Delta\dot{\mathbf{m}}$

$$S_{\delta\Gamma/\Gamma}(f) = (4\alpha/3\pi f)(\Delta\dot{\mathbf{m}}/ec)^2. \qquad (4.12)$$

To calculate the change $\Delta\dot{\mathbf{m}}$, we note that $(\dot{\mathbf{m}})^2$ is proportional to the squared transversal vibration speed of the bar and to the total mechanical energy $W=(n+1/2)\hbar\omega$ in the main oscillation mode of the resonator,

$$(n+1/2)\hbar\omega = \kappa(\dot{\mathbf{m}})^2/2. \qquad (4.13)$$

Here κ is a coefficient of proportionality easy to calculate. When a phonon is removed from the main MEMS resonator mode, the energy in Eq. (4.13) is reduced by the amount

$$\hbar\omega = \kappa\dot{\mathbf{m}}\,\Delta\dot{\mathbf{m}}\,. \qquad (4.14)$$

This yields

$$(\Delta\dot{\mathbf{m}})^2 = (\hbar\omega/\kappa\dot{\mathbf{m}})^2 = \hbar\omega/(2n+1)\kappa. \qquad (4.15)$$

Eq. (4.12) becomes now

$$S_{\delta\Gamma/\Gamma}(f) = (4\alpha/3\pi f)\hbar\omega/(2n+1)\kappa(ec^2$$
$$=\underline{4\omega/3\pi f(2n+1)\kappa c^3} = 2\hbar\omega^2/3\pi f W\kappa c^3. \qquad (4.16)$$

This quantum 1/f noise, proportional to the resonance frequency and inversely proportional to the number of quanta in the main oscillation mode, decreases when the energy in the main resonator mode increases. This is characteristic of quantum mechanical spontaneous emission noise in general. With $\langle\omega\rangle=10^{12}$ rad/sec and $W=4\ 10^{-13}$ erg we obtain about $10^{-22}/f\kappa$. The MEMS data used here are chosen arbitrarily for illustration.

To estimate the coefficient κ, we write the mechanical energy, including both the equally contributing kinetic and elastic components, in the form

$$W = M_{eff}v^2/2, \qquad (4.17)$$

where M_{eff} is a mass close to the mass M of the bar. Noting that the rate of change in the magnetic moment of the system, caused by the motion of the bar of length L with speed v, is

$$\dot{\mathbf{m}} = \mathbf{n}(I/c)dS/dt = \mathbf{n}ILv/c \qquad (4.18)$$

we find

$$\kappa = M_{eff}v^2/\dot{\mathbf{m}}^2. \qquad (4.19)$$

Using (4.18), Eq. (4.19) becomes

$$\kappa = M_{eff}[c/IL]^2. \qquad (4.20)$$

With $M_{eff}=10^{-11}$g, $L=10^{-3}$cm and $I=1$ mA, we obtain $\kappa = 10^3$ s^2cm^{-3}. Substituting into Eq. (4.16), we obtain

$$S_{\delta\Gamma/\Gamma}(f)=(4\alpha/3\pi f)(IL)^2\hbar\omega/(2n+1)M_{eff}e^2c^4$$
$$=\underline{4(IL)^2\omega/3\pi f(2n+1)M_{eff}c^5}$$
$$=2(IL)^2\hbar\omega^2/3\pi fWM_{eff}c^5 \qquad (4.21)$$

For instance, with the above numerical example, with $\omega=\langle\omega\rangle=10^{12}s^{-1}$ and with $W=10^{-13}$ erg we obtain $10^{-25}/f$.

Finally, the quantum 1/f frequency fluctuations can be obtained from the formula

$$S_{\delta\omega/\omega}=(1/4Q^4)S_{\delta\Gamma/\Gamma} \qquad (4.22)$$

which is derived in Eq. (3.5) above. This finally yields with Eq. (4.11)

$$S_{\delta\omega/\omega}=(1/2Q^4)q^2L^2\hbar\omega^2/3\pi fWM_{eff}c^3. \quad (4.23)$$

for the electrostatic capacitively coupled case, and, from Eq. (4.21),

$$S_{\delta\omega/\omega}=(1/2Q^4)(IL)^2\hbar\omega^2/3\pi fWM_{eff}c^5 \qquad (4.24)$$

for the fractional frequency fluctuation spectrum exhibited by the magnetically driven MEMS resonator. The numerical estimated show that the electrostatically driven resonator is much noisier for the same quality factor Q than the magnetically driven one, when it comes to 1/f noise. This is because the magnetic dipole radiation is much weaker, being of higher order than the electric dipole radiation.

V. CLASSICAL FORMS OF PHASE NOISE

Phase noise is generated both classically and quantum mechanically. The quantum mechanical noise source is quantum 1/f noise, which is the main subject discussed here. However, there are also classical sources of noise, investigated by Vig and Kim [20], more recently by Cleland and Rouke [21], and caused by the factors described below.

5.1. Temperature fluctuations δT are particularly important in small resonators, such as MEMS resonators, due to the "bolometer effect". In thermal equilibrium, from thermodynamics,

$$\langle(\delta T)^2\rangle = kT^2/C= kT^2/c_VV, \qquad (5.1)$$

where k is Boltzmann's constant and C the heat capacity of the resonating body, i.e., volumetric specific heat c_V, times volume V. Any temperature variations cause thermal dilatation and changes in the elastic constants and the speed of sound. These, in turn, affect the resonance frequency through the temperature coefficient $\alpha_T=d\nu/\nu dT$ of the resonance frequency ν. For silicon MEMS resonators, Nguyen [22] reported $\alpha_T=-10^{-5}$/K. Denoting by G the thermal exchange rate, we obtain

$$Cd\delta T/dt = -G\delta T;\ \ \delta T(t) = \delta T(0)\exp(-Gt/C);$$
$$\langle\delta T(t)\delta T(t+\tau)\rangle = \langle(\delta T)^2\rangle\exp(-Gt/C). \qquad (5.2)$$

Therefore, using the Wiener Khintchine theorem, the spectral densities of temperature fluctuations, of relative frequency fluctuations $y=\delta\nu/\nu$ and phase ϕ are

$$\langle(\delta T)^2\rangle_f \equiv S_{\delta T}(f) = (4kT^2/G)/[1 + (2\pi fC/G)^2], \qquad (5.3)$$

$$\langle(\delta\nu/\nu)^2\rangle_f \equiv S_{\delta\nu/\nu}(f) =(4\alpha_T^2kT^2/G)/[1 + (2\pi fC/G)^2], \quad (5.4)$$

$$\mathcal{L}(f) = (\nu^2/2f^2)S_{\delta\nu/\nu}(f)$$
$$= (\nu^2/2f^2)(4\alpha_T^2kT^2/G)/[1 + (2\pi fC/G)^2] \qquad (5.5)$$

In the case of MEMS resonators with frequencies from 100 kHz to 10 GHz, these results have been graphed by Vig and Kim [64] for heat exchange G caused by radiation, and by both radiation and conduction. Conduction turns out to be dominant in MEMS and NEMS with G between 1 and 5 x 10^{-6}, causing $\tau=C/G$ to be of the order of 10^{-5} s and smaller, so the second term in the denominator can be neglected. Thus,

$$\mathcal{L}(f) = (\nu^2/2f^2)S_{\delta\nu/\nu}(f) = (\nu^2/2f^2)(4\alpha_T^2kT^2/G)$$
$$\approx[-225 + 20\ \lg(\nu/f)]\ \text{dBc} \qquad (5.6)$$

is a good approximation.

Note that the heat conduction rate G to the support heat sink is proportional to the thickness z and width W, while inversely proportional to the length L of the resonating MEMS bar. Therefore, for self-similar scaling of the size and volume, the frequency noise spectrum will be proportional with the -1/3 power of the volume V, and the proportionality with ν^2 may introduce an additional dependence of phase noise, roughly with $V^{-2/3}$ when the same resonant mode is used. In conclusion, an inverse proportionality of classical $1/f^2$ phase noise caused by temperature fluctuations on the resonant volume V can be expected as a first rough approximation

$$\mathcal{L}(f)=(\nu^2/2f^2)S_{\delta\nu/\nu}(f) = (\nu^2/2f^2)(4\alpha_T^2kT^2/G) \approx \text{const}/V. \quad (5.7)$$

5.2. Johnson Noise, or Nyquist noise is thermal noise in the motional resistance of the vibrating crystal, i.e., in the internal friction or dissipative mechanical resistance. It is caused by the scattering of phonons out of the main resonator mode into thermal modes, both scattering on thermal phonons and on crystal defects, including also impurities and the surface. It is the thermal equilibrium noise of the same resistance that also shows fundamental quantum 1/f noise as shown here. It is given by

$$\mathcal{L}(f) = (\nu^2/2f^2)S_{\delta\nu/\nu}(f) = (\nu^2/2f^2)(kT/PQ_L^2), \quad (5.8)$$

where Q_L is the loaded Q and P is the total power dissipated in the resonator plus load. Since the product $Q\nu$ is constant at about 10^6 Hz in MEMS resonators [56],

$$\mathcal{L}(f) = (\nu^2/2f^2)S_{\delta\nu/\nu}(f) = (\nu^4/2f^2)(kT/P\nu^2Q_L^2)$$
$$\approx[40\ \lg\nu\text{-}20\ \lg f\text{-}400]\ \text{dB}, \qquad (5.9)$$

for a drive level that produces a heating of 10K of the resonator in steady state. For other drive levels, causing a heating of ΔT, 10 lg (ΔT/10) needs to be subtracted also

$$\mathcal{L}(f) = (\nu^2/2f^2)S_{\delta\nu/\nu}(f) = (\nu^4/2f^2)(kT/P\nu^2Q_L^2)$$
$$\approx[40\ \lg\nu\text{-}20\ \lg f - 10\ \lg(\Delta T/10) \text{-}400]\ \text{dB}. \qquad (5.10)$$

Here we have assumed that the heating is proportional with the drive level. The power dissipated in the resonator in stationary conditions scales with resonator volume like G, i.e., with $V^{-1/3}$, as shown in the preceding paragraph. Assuming, as is often done, that $Q_u\approx3Q_l$, we may apply this to the total dissipated power P present in Eq. (5.10). The proportionality with ν^4 may introduce an additional dependence of phase noise, roughly with $V^{-4/3}$ when the same resonant mode is used. In conclusion, an inverse 5/3 power proportionality of classical $1/f^2$ phase noise caused by Johnson (or Nyquist) noise on the resonant volume V can be expected as a first rough approximation

$$\mathcal{L}(f) = (\nu^2/2f^2)S_{\delta\nu/\nu}(f) = (\nu^4/2f^2)(kT/P\nu^2Q_L^2) \approx \text{const}/V^{5/3} \quad (5.11)$$

Comparing with the bolometer effect, Johnson noise will become important only at resonator frequencies above 10 MHz.

5.3. Acceleration noise caused by random vibration adds a phase noise contribution

$$\mathcal{L}(f) = (\nu^2/2f^2)S_{\delta\nu/\nu}(f) = \Gamma^2\langle a^2\rangle_f(\nu^2/2f^2)$$
$$= \Gamma^2 S_a(f)(\nu^2/2f^2), \qquad (5.12)$$

where Γ is the acceleration sensitivity of the resonance frequency, $\langle a^2\rangle_f = S_a(f)$ the power spectral density of the acceleration caused by external vibration to which the MEMS resonator is subjected. The factor ν^2 introduces a $V^{-2/3}$ dependence of the phase noise spectrum in this case, but S_y is independent of volume.

5.4. Total Phase Noise. By adding the classical phase noise contributions from the preceding section to a reasonable analytical form of the quantum 1/f phase noise result, we obtain the total phase noise $\mathcal{L}(f)$, with PSD of the frequency fluctuations shown inside the curly brackets and shown with a red curve as a continuation of the graph at low v in Fig. (1):

$$\mathcal{L}(f) = (\nu^2/2f^2)\{(\beta/fQ^4)/[1/V + V/\varepsilon^6] + (4\alpha_T{}^2kT^2/G)/[1 + (2\pi fC/G)^2] + (kT/Q_l{}^2P) + \Gamma^2\langle(\delta a)^2\rangle_f\}. \qquad (5.13)$$

The last 3 (classical) terms in the curly brackets are proportional to V^{-1}, $V^{-5/3}$, and $V^{-2/3}$ respectively. In terms of S_y, they are proportional to $V^{-1/3}$, V^{-1}, and V^0. They yield in terms of S_y the behavior sketched qualitatively in Fig. 1 with a red line on the left of the anthill shaped graph. The latter is predicted by the quantum 1/f theory for BAW and Si MEMS on the increasing branch of the anthill, and for SAW quartz, resonators on the decreasing branch. Note that the Q1/f anthill curve increases when the modulation frequency is lowered, so the minimum on the red curve shifts to smaller volumes. That minimum is where the lowest phase noise of Si MEMS and quartz BAW resonators is obtained through optimization.

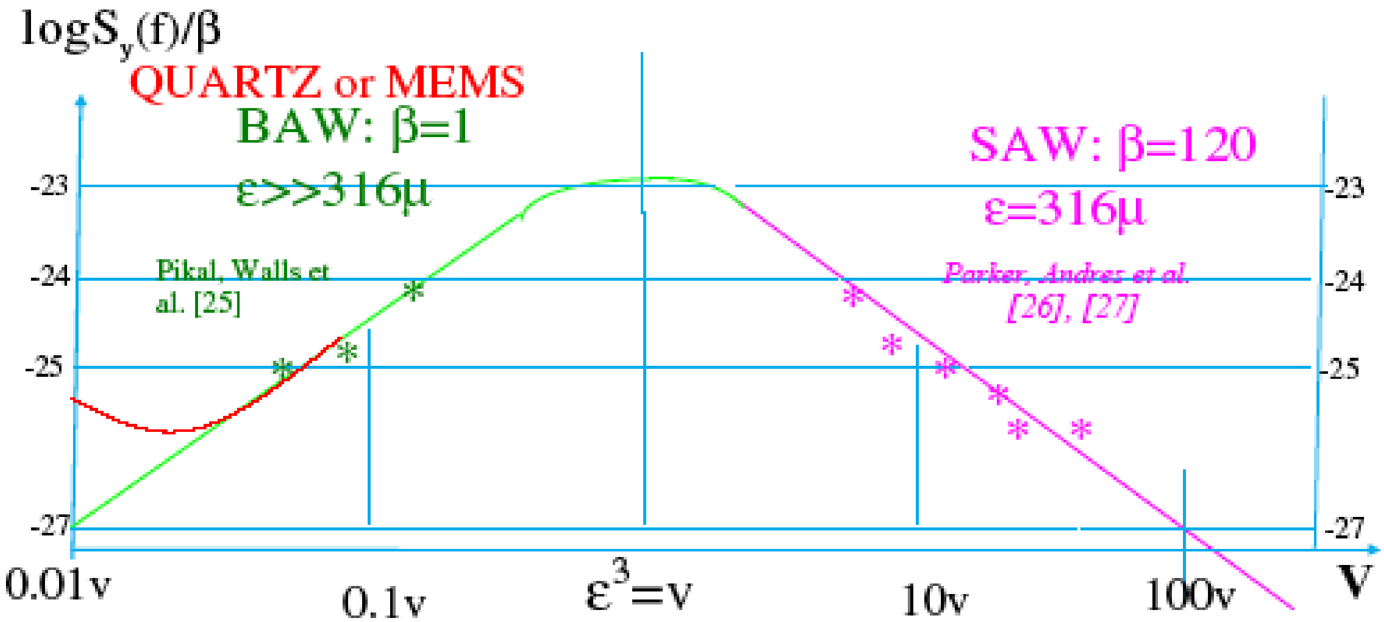


Fig. 1: Total FM noise in Si MEMS and quartz BAW & SAW resonators: the red line adds the classical white noise at small volumes.

VI. NUMERICAL ESTIMATES OF THE FREQUENCY FLUCTUATIONS SPECTRUM AND PHASE NOISE IN MEMS

J. Vig provided the examples of silicon microresonators and nanoresonators [20], shown in Table 1. These frequency and size parameters were utilized to calculate the Volume, Effective Mass, Thermal fluctuation noise, Johnson noise, and 1/f noise for the given resonator dimensions. The Thermal fluctuation and Johnson noise calculations verified the calculations of J. Vig

Eqs. (5.4) and (5.8) were used to calculate the fractional frequency fluctuation noise of Thermal fluctuation and Johnson noise respectively, while Eqs. (4.23) and eqn (4.24) were utilized to calculate the 1/f fractional frequency fluctuation noise for electrosatically and magnetically excited MEMS resonators respectively, for the given resonator volumes. The 1/f values calculated for S_y given in Table 2 range from 2.0 E^{-21} at 100 kHz to 2.3 E^{-22} at 10 GHZ, for the electrostatically excited MEMS, and in Table 3 from 2.0 E^{-25} at 100 kHz to 5.8 E^{-29} at 10 GHz, for the magnetically excited MEMS. The values of 1/f fractional frequency fluctuation noise were then converted to Phase noise with Eq. (5.8). Both the values of fractional frequency fluctuation noise and phase noise were plotted as a function of volume for both the electrostatic and magnetic excitation cases. Fig. 2 shows the plot of phase noise as a function of volume for the electrostatically excited case. The total phase noise increases as volume decreases, as was predicted theoretically. The dominant noise term shifts from 1/f noise at larger volumes to Johnson noise at small volume. This is demonstrated more clearly in Fig. 3, a plot of the fractional frequency fluctuation noise as a function of volume. The 1/f noise is the dominant term from the coherence volume until the classical Johnson noise becomes the dominant term after the frequency increases beyond the 1 GHz range. This verifies that classical noise sources dominate at the smallest size regime, below the coherence volume of a phonon (ε^3) in silicon MEMS, $\varepsilon^3 = 5\ E^{-17}\ cm^3$. Figure 4 shows the Phase noise as a function of volume for the magnetically excited MEMS resonators. The Phase noise for the magnetically excited case, also increases as volume decreases, but the 1/f contribution is never larger than the classical noise sources. The thermal noise dominates the total noise at larger volume, and the Johnson noise is the dominant term at small volume. This is shown in the graph of fractional frequency fluctuations as a function of volume for the magnetically excited MEMS, Fig 5. The 1/f noise does decrease as volume decreases, as was theoretically predicted, when Q is kept constant.

This profile of the 1/f fractional frequency fluctuation noise as a function of volume coresponds to the tail seen on the qualitative graph graph for both quartz microbalances (QCM) and MEMS resonators shown in Fig. 1. There the classical noise sources are obscured by the Q1/f noise at sufficiently low frequencies, but as the volume decreases, and as the frequency increases, the classical noise sources begin to dominate and create a noise minimum in the 1 GHz range for electrostatically excited silicon MEMS resonators. This minimum can be used to optimize the design of small and ultra-small resonators. Our analytical formulas can be used in conjunction with other analytical expressions of important system parameters in order to define a suitable figure of merit. The latter can then be optimized specifically for any given application.

VII. Discussion

Our investigation of fundamental 1/f noise has been applied to various types of quartz resonators and MEMS resonators, usually micro-fabricated from silicon. All of these resonators can be used as excellent sensors for the detection of chemical and biological agents and in general, to construct an electronic nose system, identifying trace substances by "smell." These sensors are based on the adsorption of many gas molecules (with total mass δm) on the surface of a polymer coating on the resonant element. For biological agents, corresponding antibodies are deployed on the resonant bar or disc. The adsorption gets detected by a reduction

$$y = \delta\omega/\omega = -\kappa\delta m/m \tag{7.1}$$

of the resonance frequency ω of the quartz disk. However, the latter is also subject to fundamental frequency fluctuations. Here κ is a constant of proportionality. The quantum 1/f limit of detection is given by

$$\kappa^2 S_{\delta m/m}(f) = S_y(f) = C/f;\ \ C \equiv S_y(1\text{Hz}), \tag{7.2}$$

where $S_y(f)$ is given by formulas (3.11)-(3.14) as

$$S_y(f) = \beta V/fQ^4, \text{ for } V \le \varepsilon^3;\ C = \beta V/Q^4; \tag{7.3}$$

and

$$S_y(f) = \beta\varepsilon^6/fVQ^4, \text{ for } V \ge \varepsilon^3;\ C = \beta\varepsilon^6/VQ^4; \tag{7.4}$$

as we showed in Secs. IV and V. Here V is the quartz volume (or Si MEMS volume) and C is a constant defined by Eqs. (7.3) and (7.4). Here ε^3 is the phonon coherence volume, introduced empirically by Parker et al [26]-[27] as a noise coherence volume. Usually, Eq. (7.3) is applicable to high stability BAW resonators, while Eq. (7.4) describes SAW resonators. No such simple volume dependence applies to MEMS resonators, as we can see from Eqs. (4.23) and (4.24). The Allan (two-sample) variance of y corresponding to Eq. (7.2) is known to be 2Cln2. It represents the flicker floor, i.e., the limit of the lowest attainable variance of the average y over an interval T.

TABLE I. Examples of Silicon Microresonators and Nanoresonators

Resonant Frequency	Thickness t (cm)	Width W (cm)	Length L (cm)
100 kHz	1.00E-05	4.00E-04	8.89E-03
1 MHz	1.00E-05	1.00E-04	2.81E-03
10 MHz	1.00E-05	4.00E-05	8.89E-04
100 MHz	5.00E-06	1.00E-05	1.98E-04
1 GHz	5.00E-06	5.00E-06	6.30E-05
10 GHz	1.00E-06	1.00E-06	9.00E-06
	Volume V (cm^3)	Effective Mass M_{eff} (g)	
100 kHz	3.56E-11	8.29E-11	
1 MHz	2.81E-12	6.55E-12	
10 MHz	3.56E-13	8.29E-13	
100 MHz	9.90E-15	2.31E-14	
1 GHz	1.58E-15	3.67E-15	
10 GHz	9.00E-18	2.10E-17	

Figure 2 Graph of the Phase Noise as a function of Volume for Electrostatically Excited Silicon MEMS Resonator

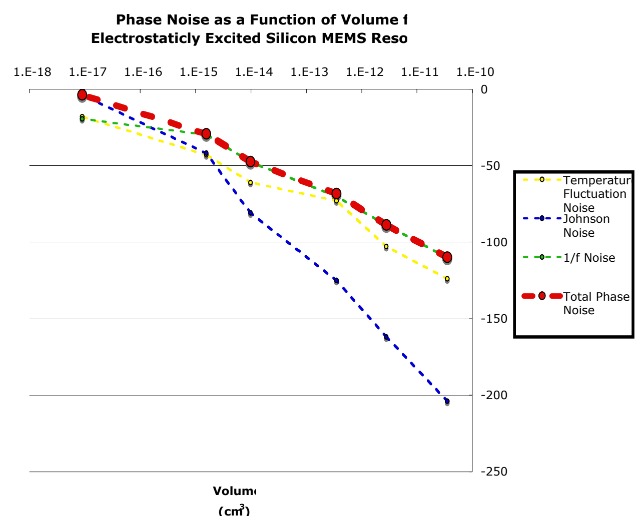


TABLE II. NOISE LEVELS FOR THE ELECTROSTATIC EXCITATION OF SILICON MEMS RESONATORS

Resonant Frequency	Temperature Fluctuation Noise		Johnson Noise	
	Phase Noise $\mathcal{L}(f)$ (dB/Hz)	Fractional Frequency Fluctuation Noise $S_y(f)$ (1/Hz)	Phase Noise $\mathcal{L}(f)$ (dB/Hz)	Fractional Frequency Fluctuation Noise $S_y(f)$ (1/Hz)
100 khz	-124	7.96E-23	-204	7.96E-31
1 Mhz	-103	1.00E-22	-162	1.26E-28
10 Mhz	-73	1.00E-21	-125	6.32E-27
100 Mhz	-61	1.59E-22	-81	1.59E-24
1 Ghz	-43	1.00E-22	-42	1.26E-22
10 Ghz	-18	3.17E-22	-4	7.96E-21
	1/f Noise		Total Noise	
	Phase Noise $\mathcal{L}(f)$ (dB/Hz)	Fractional Frequency Fluctuation Noise $S_y(f)$ (1/Hz)	Phase Noise $\mathcal{L}(f)$ (dB/Hz)	Fractional Frequency Fluctuation Noise $S_y(f)$ (1/Hz)
100 khz	-110	1.97E-21	-110	2.05E-21
1 Mhz	-89	2.49E-21	-89	2.59E-21
10 Mhz	-70	1.97E-21	-68	2.97E-21
100 Mhz	-48	3.47E-21	-47	3.63E-21
1 Ghz	-30	2.10E-21	-29	2.33E-21
10 Ghz	-19	2.31E-22	-4	8.51E-21

TABLE III. NOISE LEVELS FOR THE MAGNETIC EXCITATION OF SILICON MEMS RESONATORS

Resonant Frequency	Temperature Fluctuation Noise		Johnson Noise	
	Phase Noise $\mathcal{L}(f)$ (dB/Hz)	Fractional Frequency Fluctuation Noise $S_y(f)$ (1/Hz)	Phase Noise $\mathcal{L}(f)$ (dB/Hz)	Fractional Frequency Fluctuation Noise $S_y(f)$ (1/Hz)
100 khz	-124	7.96E-23	-204	7.96E-31
1 Mhz	-103	1.00E-22	-162	1.26E-28
10 Mhz	-73	1.00E-21	-125	6.32E-27
100 Mhz	-61	1.59E-22	-81	1.59E-24
1 Ghz	-43	1.00E-22	-42	1.26E-22
10 Ghz	-18	3.17E-22	-4	7.96E-21
	1/f Noise		Total Noise	
	Phase Noise $\mathcal{L}(f)$ (dB/Hz)	Fractional Frequency Fluctuation Noise $S_y(f)$ (1/Hz)	Phase Noise $\mathcal{L}(f)$ (dB/Hz)	Fractional Frequency Fluctuation Noise $S_y(f)$ (1/Hz)
100 khz	-150	1.98E-25	-124	7.98E-23
1 Mhz	-135	6.25E-26	-103	1.00E-22
10 Mhz	-130	1.98E-27	-73	1.00E-21
100 Mhz	-114	8.73E-28	-61	1.60E-22
1 Ghz	-110	2.12E-29	-39	2.26E-22
10 Ghz	-85	5.79E-29	-4	8.28E-21

FIGURE 3 GRAPH OF THE FRACTIONAL FREQUENCY FLUCTUATION NOISE AS A FUNCTION OF VOLUME FOR ELECTROSTATICALLY EXCITED SILICON MEMS RESONATOR

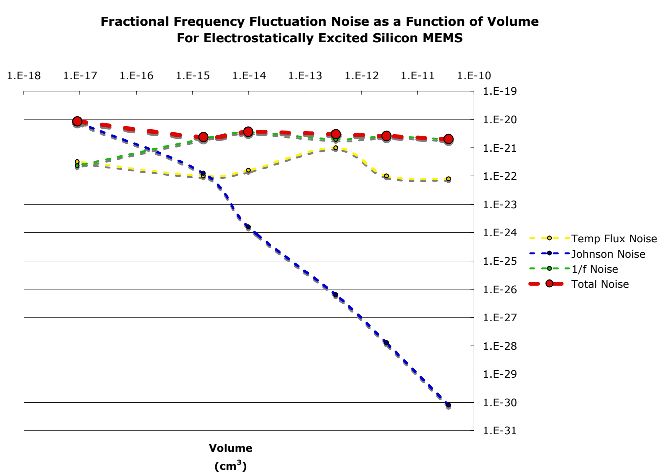


Figure 4 Graph of the Phase Noise as a function of Volume for Magnetically Excited Silicon MEMS Resonator

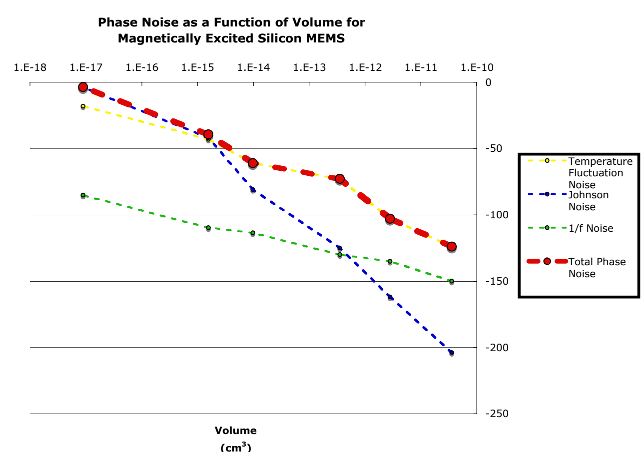
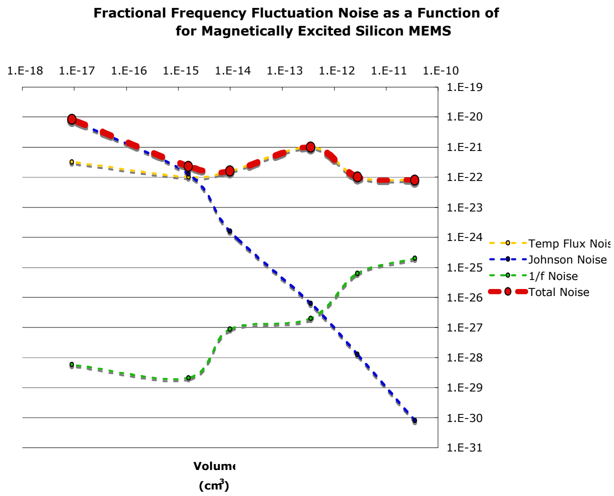


Figure 5 Graph of the Fractional Frequency Fluctuation Noise as a function of Volume for Magnetically Excited Silicon MEMS Resonator



Therefore,

$$(\delta m/m)_{min}=(2\ln 2)^{1/2}(C)^{1/2}/\kappa=(2\ln 2)^{1/2}[S_y(1Hz)]^{1/2}/\kappa \quad (7.5)$$

is the r.m.s. fractional mass deviation attainable. This result is independent of averaging time T. However, T should be larger than the averaging time τ that reduces any coexisting white frequency fluctuation noise to this limit.

To optimize the device we must avoid closeness of V with ε^3, which corresponds to the maximum error and minimal sensitivity situation. (See the graph in Fig. 1)

To reduce the measurement errors, one uses differential measurements, that include a reference resonator without polymer coating and subtract its frequency changes. This can effectively eliminate the destabilizing effect of temperature fluctuations, power supply instability, etc.

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