Quantum 1/f Noise and Phase Noise in Ferroelectrics, Piezoelectrics, MEMS Resonators, Sensors, and Piezoresponse Force Microscope

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***Abstract*—The quantum theory of 1/f noise describes the infrared-divergent conventional 1/f fluctuations of quantum mechanical cross sections and process rates by simple, universal, formulas. We give the resulting formulas for this 1/f noise and phase noise in piezoelectrics, MEMS resonators and sensors, STMs, their piezo-control loop, and currents in ferroelectrics.**

Keywords-Quantum Theory of 1/f noise; piezoelectrics; 1/f noise, MEMS, Sensors, STM, AFM, ferroelectrics

I. INTRODUCTION

The Quantum Theory of 1/f Noise is a new aspect of quantum mechanics, the time-domain consequence of the infrared divergence present in quantum electrodynamics (QED) from photons, in quantum lattice-dynamics (QLD) from piezo-phonons, in many-body physics from electron-hole pairs on the Fermi surface of metals, in quantum gravidynamics (QGD) with gravitons, etc. [1]-[5] In all acoustic transduction materials and devices, e.g., in quartz, the conventional Quantum 1/f QED form is effective. It calculates the genuine macroscopic low-frequency quantum fluctuations present in cross sections σ and process rates Γ, [1]-[5] with a 1/f spectrum:

$$\Gamma^{-2} S_{\Gamma}(f) = \frac{2\alpha A}{f} = \frac{4\alpha}{3\pi f}\left(\frac{\Delta v}{c}\right)^2$$

$$S_{\Gamma}(f) = \Gamma^2 4\alpha \left(\Delta \dot{P}\right)^2 / 3\pi e^2 c^2 f \qquad (1)$$

Here $\alpha = e^2/\hbar c = 1/137$ ($= e^2/4\pi\varepsilon_0\hbar c$ in SI) is the fine structure constant, $\Delta \mathbf{v}$ is the vector velocity change and N the num-ber of the charged particles involved in the process whose rate fluctuations we calculate, and c is the speed of light. This was verified by v.d. Ziel [6]-[8]. The second form (1) is for polarization current changes in piezo-crystals [9]-[11].

II. QUANTUM 1/f FLUCTUATIONS IN PIEZOELECTRICS

For a piezoelectric, e.g., quartz crystal resonator or sensor, there are no free charges, but the loss of a phonon causes a change $\Delta\dot{\mathbf{P}}$ in the polarization current $J = \frac{dP}{dt} = \dot{P}$.

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In Eq. (1), the rate Γ is then the rate of phonon loss from the main oscillation mode of the resonator. It will have quantum 1/f fluctuations which represent quantum fluctuations in the dissipation rate of the piezoelectric, e.g., quartz, resonator, or sensor. This also causes the fundamental 1/f fluctuations in the resonance frequency. In fact, these are quantum 1/f fluctuations in the imaginary part of the Young modulus E, and in other moduli, which can also be understood as fluctuations in the relaxation rate(s) τ.

A. Quantum 1/f Size Fluctuations

In a state with given external forces, with given stress, this will cause small macroscopic size fluctuations of the piezoelectric sample. The fractional size fluctuations of can be written in terms of the fractional fluctuations of phonon emission rate Γ

$$S_{\frac{\delta X}{X}} \approx \frac{4}{Q^4} S_{\frac{\delta\Gamma}{\Gamma}}\ ;\ S_{\frac{\delta X}{X}} \approx \frac{4}{Q^4}\left[\frac{N\alpha\hbar\langle\omega_{eff}\rangle}{3\pi nMc^2 f}\right] \qquad (2)$$

In the case that the coherence length of the phonons is smaller than the crystal size, we expect several incoherent noise contributions from various regions of the crystal. Therefore, the spectral density of fractional spatial fluctua-tions must contain the ratio of squared coherence volume and squared crystal volume

$$S_{\frac{\delta X}{X}} \approx \frac{4}{Q^4}\frac{\varepsilon^6}{V^2}\left[\frac{N\alpha\hbar\langle\omega_{eff}\rangle}{3\pi nMc^2 f}\right] = \frac{4}{Q^4}\frac{\varepsilon^6}{V}\left[\frac{(\frac{N}{V})\alpha\hbar\langle\omega_{eff}\rangle}{3\pi nMc^2 f}\right] \equiv \frac{4\beta'\varepsilon^6}{fVQ^4} \qquad (3)$$

The corresponding variance is $\frac{\delta X}{X} = \sqrt{S_{\frac{\delta X}{X}}}\,(2f\ln 2)^{1/2}$.

Here β' represents the quantity in the square brackets. In this final form, we can approximate the position fluctuations in the STM due to the phonon emission rate Γ of the piezoelectric quartz crystal that controls the feedback loop. As a first approximation, we use a phonon coherence length of 0.1mm, and a Q-factor of 100. Although the actual effective volume occupied by the mode must be used instead of the total volume between electrode, let us just assume that the piezoelectric element is a cylinder with diameter 1 cm and length 1 cm that gives a total crystal volume of 7.85 x

10^{-7} m^3. Solving $kT = \hbar < \omega_{eff} >$, we obtain $< \omega_{eff} > = 6.3 \times 10^{12}$ /s. Using a quartz lattice constant of 4.9 Å, and assuming there is only one SiO_2 molecule in the volume of the quartz unit cell, we obtain $(N/V) = 8.5 \times 10^{27}$ m^{-3}. The reduced mass of the oscillating dipoles was taken to be $M = 10^{-23}$ g. Applying these values, and substituting $n = kT/\hbar < \omega_{eff} >$ for thermal phonons, we obtain $S_{\delta X/X} = 3.6 \times 10^{-21}$ / Hz for Q = 1000 and $S_{\delta X/X} = 3.6 \times 10^{-17}$ / Hz for Q = 100. For the latter case we then get with the 2ln2=1.386 Allan variance factor mentioned above an rms size or position fluctuation of 0.72Å. This shows that for STM the position fluctuations from the piezoelectric loop are expected to be about 10 times larger than the quantum 1/f position noise with stationary needle.

B. Quantum 1/f Piezoelectric Crystal Resonance Frequency Fluctuations

For the fractional resonance frequency fluctuations caused by the quantum 1/f dissipation rate fluctuations, we obtain, as shown below,

$$S_y(f) = \frac{\beta}{f}\left(\frac{V}{Q^4}\right); \text{ with } \beta = n_0 \frac{\alpha\hbar < \omega >}{12 n\pi mc^2 \chi^2} \approx 1/cm^3 \quad (4)$$

for $V \le \varepsilon^3$. We also get

$$S(f) = \beta'\varepsilon^6/fVQ^4, \text{ for } V \ge \varepsilon^3, \quad (5)$$

as we mentioned in (3), due to the incoherence of elementary coherent domains.

To derive the frequency (and size) fluctuations, we start from the second form of (1) and find an expression for $\Delta\dot{\mathbf{P}}$. The vibrational energy of the crystal can be written in the form

$$W = n\hbar<\omega> = 2(Nm/2)(dx/dt)^2 \quad (6)$$

$$= (Nm/e^2)(edx/dt)^2 = (m/Ne^2)g^2(\dot{\mathbf{P}})^2; \quad (7)$$

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

$$\Delta n/n = 2|\Delta\dot{\mathbf{P}}|/|(\dot{\mathbf{P}}|, \text{ or } \Delta\dot{\mathbf{P}} = \dot{\mathbf{P}}/2n. \quad (8)$$

Solving (7) for $\dot{\mathbf{P}}$ and substituting into (8), we obtain

$$|\Delta\dot{\mathbf{P}}| = (N\hbar<\omega>/n)^{1/2}(e/2g). \quad (9)$$

Substituting $\Delta\dot{\mathbf{P}}$ into (1), we get

$$\Gamma^{-2}S_\Gamma(f) = N\alpha\hbar<\omega>/3n\pi mc^2 fg^2 \equiv \Lambda/f. \quad (10)$$

The dissipation rate affects the resonance frequency ω. Using the harmonic oscillator relation

$$\omega^2 = \omega_0{}^2 - 2\Gamma^2, \ \omega\delta\omega = -2\Gamma\delta\Gamma; \quad (11)$$

between resonance frequency ω and dissipation Γ, we obtain

$$S_{\delta\omega/\omega}(f) = (1/4Q^4)S_{\delta\gamma/\gamma}(f) = (1/4Q^4)(\Lambda/f)$$
$$= N\alpha\hbar<\omega>/12n\pi mc^2 fg^2Q^4; \quad (12)$$

Thus,

$$S(f) = \beta'V/fQ^4, \text{ for } V \le \varepsilon^3, \quad (13)$$

which explains (4) and (5). With an intermediary value $<\omega> = 10^{10}$/s, with $n = kT/\hbar<\omega>$, T=300K and $kT = 4 \cdot 10^{-21}$ J, we get

$$\beta' = (N/V)\alpha\hbar<\omega>/12n\pi g^2mc^2 = 10^{22}(1/137)(10^{-27}10^{10})^2$$
$$/12kT\pi 10^{-23}\, 9\, 10^{20} \approx 1. \quad (14)$$

III - QUANTUM 1/F FLUCTUATIONS IN PIEZOELECTRICS

Properly sensitized MEMS resonators are particularly useful for the un-intrusive detection of biological and chemical agents. The detection limit is proportional to the flicker floor of the resonator. The latter is given by the expression in curly brackets below. By adding the known classical phase noise contributions[1] to the quantum 1/f phase noise result derived earlier[2], we obtain the total phase noise L(f), with PSD of the frequency fluctuations shown inside the curly brackets and shown with a red curve in Fig. (1) below

$$L(f) = (v^2/2f^2)\{(\beta/fQ^4)/[1/V + V/\varepsilon^6] + (4\alpha_T^2kT^2/G)/[1 +$$
$$(2\pi fC/G)^2] + (kT/Q_L{}^2P) + \Gamma^2<(\delta a)^2>_f\}. \quad (15)$$

Dividing by $(2\pi)^2$, and expressing in dB, we obtain it in dBc. The spectral density $S_y(f)$ of fractional frequency fluctuations $\delta v/v$ is the expression in curly brackets. Here v is the MEMS vibration frequency, β the quantum 1/f coefficient, V the effective volume of the oscillating finger or bar, ε the phonon coherence length in the (silicon) MEMS material, $\alpha_T = dv/vdT$ the temperature coefficient of the resonance frequency v. G is the thermal exchange rate and C the heat capacity of the oscillating volume. Q_L is the loaded Q and P is the total power dissipated in the resonator plus load. Finally, Γ is the acceleration sensitivity of the resonance frequency, $<a^2>_f = S_a(f)$ the power spectral density of the acceleration caused by external vibration to which the MEMS resonator is subjected. The last 3 (classical) terms in the curly brackets are proportional to V^{-1}, $V^{-5/3}$, and $V^{-2/3}$ respectively, and yield the behavior sketched qualitatively in Fig. 1 below with a red line on the known[2] ant-hill 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.*

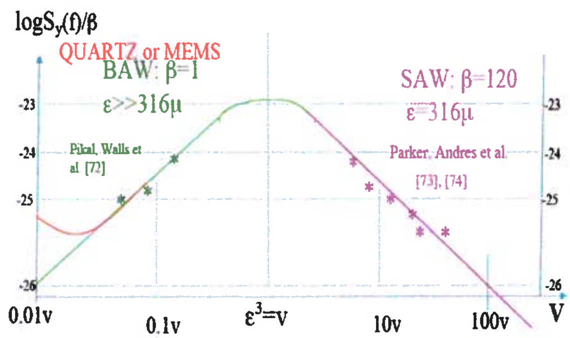

Fig. 1: Total FM noise in Si MEMS and quartz BAW & SAW resonators: the red line adds the classical white noise at small volumes.

IV. Quantum 1/f Noise in STM

When the needle is stationary, we may be able to avoid the noise of the piezoelectric feedback loop. Then we will notice the quantum 1/f noise in the needle, in the vacuum between needle and sample, and the noise in the spreading resistance in the sample. We briefly provide here our result.

In the tungsten tip, a preliminary calculation of the coherence parameter s indicated that both coherent and conventional quantum 1/f effects affect the resistance, with weights determined by the coherence parameter $s = 5.6 \cdot 10^{-13}$ cmN'; Here N' is the number of electrons per cm in the direction of the current. A detailed calculation of the 1/f noise contributions in the tip yields analytical expressions for the spectral density of fractional resistance fluctuations $\delta R_t/R_t$. For a tungsten tip cone angle of 7.5°, minimal radius of 100Å, total length of 15 μ, one obtains $S_{dRt/Rt} \cong 10^{-10}/f$.

In the vacuum through which the electrons tunnel, s<<1 and only conventional quantum 1/f effect is present. We obtain in this case, with a potential barrier of U=0.1 eV, tunneling current of 20 pA, and a tunneling gap of $3 \cdot 10^{-10}$ m, possibly modulated by a chemical agent's molecules that are studied,

$$S_{\delta R_v/R_v}(f) = \frac{4\alpha}{3\pi f N}\frac{(\Delta v)^2}{c^2}; \quad S_{\delta R_v/R_v} = \frac{4.8 \cdot 10^{-8}}{f} \qquad (16)$$

In the sample, the quantum 1/f effect in the spreading resistance is mainly coherent, with small conventional contributions. The sample in [12] is taken to be a silver film, thickness 50 nm, evaporated on a silicon wafer.

$$S_{\delta R_s}(f) = \frac{1}{1+s} S^{conv}_{\frac{\delta R_s}{R_s}}(f) \cdot R_s^2 + \frac{s}{1+s} S^{coh}_{\frac{\delta R_s}{R_s}}(f) \cdot R_s^2$$

$$= \int_{r_i}^{r_f} \frac{1}{1+s}\left(\frac{4\alpha\left(\frac{\Delta v}{c}\right)^2}{3\pi f \cdot dN}\right)\left(\frac{\rho_{Au} dr}{2\pi r^2}\right)^2 + \int_{r_i}^{r_f} \frac{s}{1+s}\left(\frac{2\alpha}{\pi f \cdot dN}\right)\left(\frac{\rho_{Au} dr}{2\pi r^2}\right)^2$$

$$S = \frac{5.6 \cdot 10^{-5}\,\Omega^2}{f}. \qquad (17)$$

Within the silver sample we have a number of electrons $dN = n_{Ag} dV = n_{Ag} 2\pi r^2 dr$, in a hemispherical shell of thickness dr, and the coherence parameter is $s = N' r_o = 4\pi r_o n_{Ag} r^2$; here $r_o = e^2/mc^2 = 2.8 \; 10^{-13}$ cm = classical radius of the electron, N' is the number of electrons per cm.

The total resulting resistance R (and current at constant applied V) fluctuations are thus given by tip, vacuum and sample contributions:

$$S_{\frac{\delta R}{R}}(f) = S_{\frac{\delta I}{I}}(f) \qquad (3)$$

$$= \left(\frac{R_t}{R}\right)^2 S_{\frac{\delta R_t}{R_t}}(f) + \left(\frac{R_v}{R_{total}}\right)^2 S_{\frac{\delta R_v}{R_v}}(f) + \left(\frac{R_s}{R_{total}}\right)^2 S_{\frac{\delta R_s}{R_s}}(f) = \frac{4.8 \cdot 10^{-8}}{f}$$

With a tunneling exponent per unit length $\kappa = [(2mU)^{1/2}]/\hbar$, and quality factor of the THz oscillation loop $Q_l = 10$, this yields an error ds_o in the determination of the height of the sample, and a frequency noise $S_{\delta\omega/\omega}$ for STM THz signatures

$$\delta s_0 = \frac{\delta I}{I}\frac{1}{2\kappa} = \sqrt{\frac{4.8x10^{-8}}{f}}\left(\frac{1}{2\left(\frac{20}{1x10^{-9}m}\right)}\right) = \frac{5.5x10^{-15}m}{\sqrt{Hz}} \qquad (19)$$

$S_{\delta\omega/\omega} = (S_R/R^2)/4Q_l^4 f = 4.8 \cdot 10^{-8}/4 \cdot 10^4 f = 1.2 \cdot 10^{-12}/f = C/f$, (20)

The achievable rms THz spectral resolution is therefore, $\Delta\omega/\omega = [2\,C\,\ln 2]^{1/2} = [2\ln 2(S_R/R^2)/4Q_l^4]^{1/2} = [1.66 \cdot 10^{-12}]^{1/2}$, which correspond to a phase noise

$\mathcal{L}(f) = 10\log[(1/2)(\omega/2\pi f)^2 S_{\delta\omega/\omega}(f)] = 27$ dBc at f=1 kHz, for $\omega/2\pi = 1$ THz.

In the theoretical quantum 1/f calculation of the current noise, the dominant term was found to be the noise from the tunneling current. The corresponding current fluctuations, δI, are $4.3 \cdot 10^{-15} \cdot (2\ln 2)^{1/2}$, or in amplitude

$$\delta I = \sqrt{S_{\delta I}} = 4.3x10^{-15}\frac{A}{\sqrt{Hz}}. \qquad (21)$$

The experimental data of Koslowski [12] for the magnitude of the tunneling current noise was obtained by two methods; using a digital signal analyzer connected to the current signal to precisely measure the spectral behavior and using a crude 'noisemeter' consisting of two independent channels that evaluate the noise magnitude at two specific frequencies f_1 = 2.3 kHz and f_2 = 4.7 kHz. These two frequencies were chosen to be well above the cutoff frequency of the topographic feedback loop to avoid interference from the current noise and other properties of the feedback loop, such as the tunneling barrier height. Each channel of the 'noisemeter' calculates the noise magnitude by passing the current signal through a bandpass filter. The filter signal is then squared and averaged over a time interval switchable between about 30 ms or 300ms. The output signal of the 'noisemeter' is proportional to the power spectral density of the current noise at 2.3 or 4.7 kHz.

The experiments were done on thin silver films deposited onto silicon. In surface images, the bright areas were defined as regions of high current noise (later referred to as S regions) embedded in darker regions of low current noise (M regions). At the 2.3 kHz frequency, the spectral density of current noise in the M regions was approximately $S_I = 1.2 \times 10^{-27}\ A^2 / Hz$ and in the S regions approximately $S_I = 2 \times 10^{-25}\ A^2 / Hz$. The corresponding noise amplitudes are obtained by taking square roots, as above, giving the current fluctuations δI. In the low noise regions this gives $\delta I = 3.5 \times 10^{-14}$ and for high noise regions $\delta I = 4.5 \times 10^{-13}$.

The theoretical noise amplitudes are fairly close to the observed values in the low noise regions of the sample, within one order of magnitude. The theoretical values obtained were based on geometrical parameters that were estimated, such as tip geometry, tip-sample separation distance, and current set by the feedback loop.

The achievable THz spectral resolution for STM chemical agent identification from their THz signature is thus,

$$\Delta\omega/\omega=[2C\ln 2]^{1/2}=[2\ln 2(S_R/R^2)/4Q_I^4]^{1/2}$$
$$=[1.66\cdot 10^{-12}]^{1/2}=\underline{1.3\ 10^{-6}} \qquad (22)$$

This expression allows for the optimization of the system by optimizing the factors contained in the expression of S_R/R^2.

For instance, the noise is reduced if the velocity change of the electrons in the tunneling process is lowered, thereby reducing the bremsstrahlung amplitude of this process. This amplitude determines the conventional part of quantum 1/f noise. It also would be useful to increase the number of electrons involved in tunneling at any time, so N would be larger than 1 in Eqs. (48)-(49). A reviewer has suggested the use of a gas instead of vacuum, in order to increase N. This, however, introduces other forms of noise caused by the fluctuating number of adsorbed gas molecules on the sample and tip surfaces. If this problem could be overcome with the use of noble gases, the formation of space charge would also help to reduce noise. This would in fact sacrifice lateral spatial STM resolution for sharper spectral sensing of chemical and biological agents.

We finally mention that the data characterizing various STM systems could differ very much from what we used as an example. For instance, if instead of using k=20/nm in the exponent of the tunneling transmission factor we would use the higher value of 25/nm, the vacuum resistance would increase its exponent of 9 by about 20%, i.e., the current would decrease by almost 2 orders of magnitude. On the other hand, a tenfold increase in the quality factor of 10 that was assumed at THz frequencies, would decrease the frequency uncertainty $\Delta\omega/\omega$ by 2 orders of magnitude.

V. Verification of Quantum 1/f Phase Noise in Quartz

In 1992 F.L. Walls [13] verified for the first time the unexpected quantum 1/f prediction of increase in phase noise close to carrier in small high stability BAW quartz resonators proportional with the volume, shown in (4) and (13). More recently, after a five-year study, F. Sthal et.al. [14]-[15] found in great detail how exactly the quantum 1/f formulas and anthill-shaped graph apply to quartz resonators.

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