1/f Noise in a Coulomb Glass

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At low temperatures electron hopping in a three dimensional Coulomb glass produces fluctuations in the single particle density of states and hence in the resistivity. This results in a low frequency resistivity noise spectrum which goes as $f^{-\alpha}$ where $\alpha$ is very close to 1. This holds down to extremely low frequencies.

Low frequency 1/f noise is ubiquitous; it is found in a wide variety of conducting systems such as metals, semiconductors, tunnel junctions, and even superconducting SQUIDs. Yet the microscopic mechanisms are still not well understood. In some cases the electrons are in a Coulomb glass which is an insulator with randomly placed electrons that have Coulomb interactions. Lightly doped semiconductors and disordered metals are examples of such systems. This paper focuses on 1/f noise in Coulomb glasses. Experimental studies on doped silicon inversion layers have shown that low frequency 1/f noise is produced by hopping conduction. More recent experiments have observed 1/f noise down to 0.1 Hz in boron–doped silicon. Because the systems are glassy, electron hopping can occur on very long time scales and this produces low frequency noise. In this paper we show that the resulting noise spectrum goes as $f^{-\alpha}$ where $f$ is frequency and the exponent $\alpha \approx 1$.

Shklovskii developed the first theory of 1/f noise in Coulomb glasses. He suggested that it is produced by fluctuations in the number of electrons in an infinite percolating cluster. These fluctuations are caused by the slow exchange of electrons between the infinite conducting cluster and small isolated donor clusters. A more rigorous calculation combined with numerical simulations of Shklovskii’s model found a noise spectrum that went as $f^{-\alpha}$ where $\alpha$ was considerably lower than 1. Furthermore, below a minimum frequency of order 1–100 Hz, the noise spectral density saturated and became a constant independent of frequency. A similar conclusion holds for a model suggested by Kozub in which electron hops within finite clusters produce fluctuations in the potential seen by hopping conduction electrons that contribute to the current. Kogan has argued that transitions between valleys in the energy landscape produces 1/f noise because high barriers result in slow fluctuations in hopping conduction.

In our approach electron hopping shifts the single particle energies $\varepsilon$ because they depend on Coulomb interactions with other sites. This leads to fluctuations in the single particle density of states $g(\varepsilon)$ which, in turn, produce fluctuations in the conductivity. The conductivity depends on the density of states $g(\varepsilon \approx \mu)$ in the vicinity of the Fermi energy $\mu$. Note that $g(\varepsilon \approx \mu)$ can be affected by hops between sites $i$ and $j$ even if the energies on these sites are not near the Fermi energy because an electron or hole on site $i$ or $j$ can interact with other sites whose energy is (or was) near the Fermi energy.

We start with a model of the Coulomb glass that follows that of Baranovskii, Shklovskii, and Efros (BSE). In this model, the electrons occupy the sites of a periodic lattice, and the number of electrons is half the number of sites. Each site has a random onsite energy $\phi_i$ chosen from a uniform distribution extending from $-A$ to $A$. Thus, $g_0$, the density of states without interactions, is flat. A site can contain 0 or 1 electron. The Hamiltonian can be written as:

$$H = \sum_i \phi_i n_i + \sum_{i>j} \frac{e^2}{\kappa r_{ij}} n_i n_j$$

(1)

where the occupation number $n_i$ equals $\frac{1}{2}$ if site $i$ is occupied and $\frac{1}{2}$ if site $i$ is unoccupied, $\epsilon$ is the electron charge, $\kappa$ is the dielectric constant and $r_{ij}$ is the distance between sites $i$ and $j$. The single site energy is $\epsilon_i = \phi_i + \sum_j \frac{e^2}{\kappa r_{ij}} n_j$. At zero temperature Coulomb interactions between localized electrons result in a so-called Coulomb gap in the single particle density of states that is centered at the Fermi energy.

We will use Mott’s argument for variable range hopping to relate fluctuations in the density of states to fluctuations in the resistivity. One can regard a Coulomb glass as a random resistor network with a transition between sites $i$ and $j$ associated with a resistance $R_{ij}$ given by:

$$R_{ij} = R_0^\alpha \exp(\xi_{ij})$$

(2)

where the prefactor $R_0^\alpha = kT/(e^2 \gamma_{ij}^\alpha)$ with $\gamma_{ij}^\alpha$ given by:

$$\gamma_{ij}^\alpha = \frac{D^2 |\Delta_i|}{\pi d s^5 h^2} \left[ \frac{2e^2}{3\kappa a} \right]^2 \frac{r_{ij}}{a^2} \left[ 1 + \left( \frac{\Delta_i a}{2\hbar s} \right)^2 \right]^{-4}$$

(3)

where $D$ is the deformation potential, $s$ is the speed of sound, $d$ is the mass density, and $\Delta_i = \varepsilon_j - \varepsilon_i - e^2/\kappa r_{ij}$. $\Delta_i$ is the change in energy that results from hopping from
$i$ to $j$. $a = \kappa a_B$ is the effective Bohr radius of a donor, and $a_B$ is the usual Bohr radius ($a_B = \hbar^2/m e^2$). We will set the mass $m$ equal to the electron mass so that $a_B = 0.529\text{\AA}$. In eq. (3), the exponent is given by
\[ \xi_{ij} = \frac{2r_{ij}}{a} + \frac{\varepsilon_{ij}}{kT}. \] (4)

The exponent reflects the thermally activated hopping rate between $i$ and $j$ as well as the wavefunction overlap between the sites. $\varepsilon_{ij}$ is given by [3]:
\[ \varepsilon_{ij} = \left\{ \begin{array}{lr} |\varepsilon_i - \varepsilon_j| - \frac{2}{|C|}, & (\varepsilon_i - \mu)(\varepsilon_j - \mu) < 0 \\ \max[|\varepsilon_i - \mu|,|\varepsilon_j - \mu|], & (\varepsilon_i - \mu)(\varepsilon_j - \mu) > 0 \end{array} \right. \] (5)

At both high and low compensations, electron hopping usually occurs on one side of the Fermi level $\mu$ and the lower expression applies. At intermediate compensations and in the regime of variable range hopping, hopping electrons often cross the Fermi level and the upper expression applies.

In the regime of variable range hopping Mott pointed out that hopping conduction at low temperatures comes from states near the Fermi energy. Let $\bar{\varepsilon} = \varepsilon - \mu$. If we consider states within $\varepsilon_o$ of the Fermi energy, then the concentration of states in this band is $N(\varepsilon_o) = \int_{-\varepsilon_o}^{\varepsilon_o} g(\bar{\varepsilon})d\bar{\varepsilon}$ where $g(\bar{\varepsilon})$ is the density of states measured from the Fermi energy. So the typical separation between sites is $R = [N(\varepsilon_o)]^{-1/3}$. To estimate the resistance corresponding to hopping between two typical states of the band, we replace $r_{ij}$ with $R$ and $|\varepsilon_j - \varepsilon_i|$ with $\varepsilon_o$ in eqs. (1) and (3) to obtain $\xi(\varepsilon_o)$. Minimizing $\xi(\varepsilon_o)$ yields $\varepsilon_o$. Plugging this into eqs. (1) and (3) yields the variable range hopping formula for the resistivity $\rho(T) = \rho_o(T) \exp(\xi(\varepsilon_o))$.

In our model the noise results from electron hopping which produces fluctuations in the density of states $g(\varepsilon) = \overline{g}(\varepsilon) + \delta g(\varepsilon)$, where $\overline{g}(\varepsilon)$ is the average density of states. This in turn creates fluctuations in $N(\varepsilon_o), \xi(\varepsilon_o), \varepsilon_o$, and $\rho(T)$. We can calculate these fluctuations by applying classical perturbation theory [24] to the derivation of the variable range formula. To first order, $\delta(\varepsilon_o) = \delta\rho(T)/\overline{\rho}(T) = -(2kTg(\varepsilon_o)\varepsilon_o)^{-1} \int_{-\varepsilon_o}^{\varepsilon_o} \delta g(T, \varepsilon) d\varepsilon$. We have included the temperature dependence of the density of states because at finite temperatures the Coulomb gap fills in and the density of states no longer vanishes at the Fermi energy [21, 22]. The autocorrelation function for the fluctuations in the resistivity is
\[ \frac{\langle \delta \rho(T, t_2)\delta \rho(T, t_1) \rangle}{\overline{\rho}^2(T)} = \frac{1}{4k^2Tg^2(T, \varepsilon_o)} \int_{-\varepsilon_o}^{\varepsilon_o} d\varepsilon \int_{-\varepsilon_o}^{\varepsilon_o} d\varepsilon' \langle \delta g(T, \varepsilon, t_2)\delta g(T, \varepsilon', t_1) \rangle \] (6)

We assume that there is no correlation between the fluctuations in the density of states at different energies, so $\langle \delta g(T, \varepsilon, t_2)\delta g(T, \varepsilon', t_1) \rangle = E < \delta g(T, \varepsilon, t_2)\delta g(T, \varepsilon, t_1) > \delta(\varepsilon - \varepsilon')$ (7)

where $E$ is an energy of order $2\varepsilon_o$. Furthermore we assume that the time and energy dependence of the density of states autocorrelation function are separable, allowing us to write
\[ \int_{-\varepsilon_o}^{\varepsilon_o} d\varepsilon \langle \delta g(T, \varepsilon, t_2)\delta g(T, \varepsilon, t_1) \rangle = C(\varepsilon_o, T)f(T, t_2 - t_1) \] (8)

where we are assuming translational invariance in time (stationary processes). $C(\varepsilon_o, T)$ is a function of $\varepsilon_o$ and temperature. The function $f(T, t)$ characterizes the time dependence of the return to equilibrium by the system after it is perturbed by a fluctuation in the density of states. Inserting eqns. (7) and (8) in (6) yields
\[ \frac{\langle \delta \rho(T, t_2)\delta \rho(T, t_1) \rangle}{\overline{\rho}^2(T)} = \frac{EC(\varepsilon_o, T)}{4k^2T^2g^2(T, \varepsilon_o)} f(T, t_2 - t_1) \] (9)

To relate this to the spectral density of the noise $S(\omega)$, let $\psi_\omega(t_2 - t_1) = \langle \delta \rho(T, t_2)\delta \rho(T, t_1) \rangle$ and let $\psi_\rho(\omega)$ be the Fourier transform of $\psi_\omega(t_2 - t_1)$. According to the Wiener–Khinchin theorem [2], for a stationary process the spectral density of fluctuations is given by [27]
\[ S_\rho(\omega) = 2\psi_\rho(\omega) = \frac{EC(\varepsilon_o, T)}{2k^2T^2g^2(T, \varepsilon_o)} f(T, \omega) \] (10)

We do not know the temperature dependence of $f(T, t)$, so for the moment we will suppress this and just refer to $f(t)$. Theoretical calculations find that after large deviations from equilibrium, the density of states returns to equilibrium with a time dependence given by $g(\mu, t) \sim -\ln t$ or $g(\mu, t) \sim t^{-\theta}$ where $\theta \ll 1$ [28]. This agrees with experiments done at low temperatures [29, 31]. If we assume that these functional forms are also valid for $f(t)$ which applies to small perturbations, then we obtain $1/f$ noise. We now describe the calculation leading to this conclusion [28]. One starts with the Hamiltonian (1) but assumes that the Coulomb interactions are turned on at time $t = 0$:
\[ H = \sum_i \phi_i n_i + \sum_{i > j} \frac{e^2}{\kappa^2r_{ij}} n_in_j \theta(t) \] (11)

where the step function $\theta(t)$ is 0 for $t < 0$ and 1 for $t \geq 0$. So for $t < 0$ the noninteracting density of states is a constant $g_o$. Once the interactions are turned on, one follows the subsequent time development of the Coulomb gap.
The Coulomb gap arises because the stability of the ground state with respect to single electron hopping from an occupied site \( i \) to an unoccupied site \( j \) requires \( \Delta_i^f > 0 \). So we need to subtract from the density of states those states which violate this stability condition. This leads to a self-consistent equation for the density of states [4][28][32]:

\[
g(\tilde{\epsilon}, t) = g_0 \prod_{j > i} \left( 1 - a_0^3 \int_{-A}^{A} d\epsilon' g(\tilde{\epsilon}', t) \theta(\epsilon'^2_{ij} + \tilde{\epsilon} - \tilde{\epsilon}') \right)
\]

\[
F(n'_i = 1, n'_j = 0) \theta(t - \tau_{ij}(\tilde{\epsilon}', \tilde{\epsilon}, r_{ij})) \right) \tag{12}
\]

where the single-site energy \( \tilde{\epsilon}_i = \tilde{\epsilon} \), \( \tilde{\epsilon}_j = \tilde{\epsilon}' \), and \( a_0 \) is the lattice constant. \( n'_i = n_i + 1/2 \); so \( n'_i = 1 \) if site \( i \) is occupied and 0 if site \( i \) is unoccupied. \( F(n'_i, n'_j) \) is the probability that donors \( i \) and \( j \) have occupation numbers \( n'_i \) and \( n'_j \), respectively, while all other sites have their ground state occupation numbers \( \tilde{n}_k \). \( \tau_{ij}^{-1} \) is the number of electrons which jump from site \( i \) to site \( j \) per unit time. \( \theta(t - \tau_{ij}) \) represents the fact that at time \( t \), the primary contributions to the change in the density of states will be from those hops for which \( \tau_{ij} < t \). In writing eq. [13], we assume that these hops together with phonons have equilibrated the system as much as is possible at time \( t \). The hopping rate \( \tau_{ij}^{-1} \) is given by [7]

\[
\tau_{ij}^{-1} = \gamma_{ij}^o \exp(-\frac{2\tau_{ij}}{a})[1 + N(\Delta_i^f)]F(n'_i = 1, n'_j = 0) \tag{13}
\]

where \( N(\Delta_i^f) \) is the phonon occupation factor and reflects the contribution of phonon assisted hopping. We are also allowing for spontaneous emission of phonons since we are considering a nonequilibrium situation in which electrons hop in order to lower their energy. Following [4][28] we can rewrite the self-consistent equation \( g(\tilde{\epsilon}, t) \):

\[
g(\tilde{\epsilon}, t) = g_0 \exp \left\{ -\frac{1}{2} \int_{-A}^{A} \int_{-A}^{A} \frac{d\epsilon' d\epsilon''}{\alpha} \int_{-\infty}^{\infty} dr d4\pi r^2 \right\}
\]

\[
F(n(\tilde{\epsilon}) = 1, n(\tilde{\epsilon}') = 0) \theta(\epsilon'^2_{ij} + \tilde{\epsilon} - \tilde{\epsilon}') \theta(t - \tau(\tilde{\epsilon}', \tilde{\epsilon}, r)) \right) \tag{14}
\]

At low energies large distances play an important role and so we have replaced the sum by an integral over \( r \) in the exponent. The origin is at site \( i \). \( n(\tilde{\epsilon}) \) is the occupation probability of a site with energy \( \tilde{\epsilon} \). \( \tau(\tilde{\epsilon}', \tilde{\epsilon}, r) \) is given by [13] with \( r_{ij} \) replaced by \( r \), \( \tilde{\epsilon}_i \) replaced by \( \tilde{\epsilon} \), and \( \tilde{\epsilon}_j \) replaced by \( \tilde{\epsilon}' \).

Since it is not clear how the stability condition \( \Delta_i^f > 0 \) can be applied to finite temperatures, we confine our calculations to the case of \( T = 0 \). In this case the phonon occupation factor \( N(\Delta_i^f) = 0 \) and the electron occupation factor \( F(n_i = 1, n_j = 0) = 1 \) if \( \tilde{\epsilon}_i < 0 \) and \( \tilde{\epsilon}_j > 0 \). Otherwise \( F(n_i = 1, n_j = 0) = 0 \). We can solve eq. (14) iteratively on the computer. After a few iterations the typical difference between successive iterations is typically less than 1 part in \( 10^4 \). We find that the Coulomb gap develops slowly over many decades in time [28]. After an infinite amount of time, the density of states at the Fermi energy \( \mu \) goes to zero and \( g(\tilde{\epsilon}) \sim \tilde{\epsilon}^2 \).

The functional form of the time dependence of \( g(\tilde{\epsilon}, t) \) varies with the energy \( \tilde{\epsilon} \) and with \( g_o \). For conduction noise we are interested in the time dependence of the density of states at the Fermi energy which is shown in Figure [4] for \( 10^{-8} < t < 10^8 \) s. For \( g_o = 2 \times 10^5 \) states/K–Å\(^3\), we can fit our results to the form \( g(\mu, t) = B_1 \ln(t_o/t) \) where \( t < t_o, t_o \approx 3 \times 10^{43} \) sec, and for \( g_o = 6.25 \times 10^5 \) states/K–Å\(^3\), \( g(\mu, t) \approx B_2 t^{-\theta} \) where \( \theta \approx 0.05 \). The values of \( B_1, B_2 \), and the other parameters used to obtain these results are given in the caption of Figure [4]. These fits change slightly for longer times. For example, for \( 10^{-8} < t < 10^{100} \) s and \( g_o = 2 \times 10^5 \) states/K–Å\(^3\), the fit to our results has the form \( g(\mu, t) \sim t^{-\theta} \) where \( \theta \approx 0.01 \). Still we see that the density of states at the Fermi energy approaches its equilibrium value roughly logarithmically in time. This is consistent with recent experiments on thin semiconducting [28,31] and metallic [37] films which have shown that the system adjusted to changes in the Fermi energy approximately logarithmically in time. These films were grown on insulating substrates which separated them from a gate electrode that regulated the electron density, and hence the chemical potential, of the film. The conductance was measured as a function of the gate voltage. If the gate voltage was changed suddenly from, say, \( V_o \) to \( V_1 \), the conductance had a very fast initial rise, followed by a period of rapid relaxation, which in turn was followed by a long period of very slow relaxation. The relaxation could be described by \( \ln t \) or \( t^{-\theta} \) with \( \theta \) being small and varying slowly with time. This is consistent with our view [28] that when the gate voltage is changed, the Fermi energy changes, and time dependent relaxations arise because the system must dig a new Coulomb gap in the density of states at the new Fermi energy.

So both theory and experiment indicate that the nonequilibrium density of states approaches its equilibrium value roughly logarithmically in time. Returning to the original model described by [4], we assume that this time dependence holds true in the linear response regime at low temperatures. If a fluctuation \( \delta g(\mu, t = 0) \) at \( t = 0 \) pushes the density of states away from its mean equilibrium value at the Fermi energy, then this perturbation will decay according to \( f(t) \) which enters into eqs. (8) and (9). Our nonequilibrium calculation indicates that \( f(t) \) can have the form:

\[
f_1(t) = B_1 \ln(t_o/t) \tag{15}
\]

where \( t < t_o \), and \( t_o \) is on the order of the age of the universe or longer, or
\[ f_2(t) = B_2 t^{-\theta} \]  
(16)

where \( \theta \ll 1 \), and \( B_1 \) and \( B_2 \) are positive constants of order \( g_0 \). In both cases \( t \) is greater than some \( t_{\text{min}} \) of order \( 10^{-8} \) s, say. The time dependence is a function of the energy, so here we set \( \varepsilon = \mu \). Fourier transforming \( f_1(t) \) and keeping the real part, we find that

\[ f_1(\omega) \approx \frac{\pi B_1}{2\omega} \]  
(17)

This implies that the noise spectral density \( S(\omega) \sim 1/\omega \). Fourier transforming \( f_2(t) \) and keeping the real part yields

\[ f_2(\omega) \approx \frac{\pi B_2 \theta}{2\omega^{1-\theta}} \]  
(18)

for \( \theta \ll 1 \). This implies \( S(\omega) \sim 1/\omega^{1-\theta} \). To summarize, electron hopping leads to fluctuations in the density of states that relax back to equilibrium roughly logarithmically in time. This leads to 1/f noise in the spectral density \( S(\omega) \) of the noise in the resistivity. In particular we find that \( S(\omega) \sim 1/\omega^\alpha \), where \( \alpha = 1 \) if the relaxation is logarithmic in time, and \( \alpha = 1 - \theta \) if the relaxation is a power law that goes as \( t^{-\theta} \) where \( \theta \ll 1 \). In general \( \alpha \) depends on temperature and is weakly dependent on the noninteracting density of states \( g_0 \) and on the times scales. As eq. (10) indicates, the noise amplitude also depends on the temperature. Unfortunately we cannot ascertain these temperature dependencies because we do not know the temperature dependence of the fluctuations \( \delta g(T, \varepsilon, t) \) in the density of states. However we believe that our mechanism for 1/f noise should be valid at low temperatures \( (T \gtrsim 20 \text{ K}) \) where the logarithmic time dependence of the conductance is observed after the Coulomb glass has been pushed out of equilibrium by the sudden application of a gate voltage.

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FIG. 1. Density of states \(g(\varepsilon = \mu, t)\) at the Fermi energy as a function of time for different values of \(g_0\). Solid lines are fits to the numerical integration of (14). The fit to the \(g_0 = 2 \times 10^5\) states/K–Å\(^3\) data is given by \(B_1 \ln(t_o/t)\) where \(\ln t_o = 100\) with time measured in seconds and \(B_1 = 1.64 \times 10^{-7}\) states/K–Å\(^3\). The fit to the \(g_0 = 6.25 \times 10^5\) states/K–Å\(^3\) data is given by \(B_2 t^{-\theta}\) where \(\theta = 0.050\) and \(B_2 = 1.82 \times 10^{-5}\) states/K–Å\(^3\). Parameters used are \(A = 2 \times 10^4\) K, \(\kappa = 10\), \(d = 7.18\) g/cm\(^3\), \(s = 5.0 \times 10^5\) cm/sec, \(D = 5 \times 10^3\) K, and \(a_o = 4\) Å. The density \(d\) is chosen to be that of In\(_2\)O\(_3\).