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Possible mechanisms for $1/f$ noise in chalcogenide glasses: A theoretical description

M. Nardone
Department of Physics and Astronomy, University of Toledo, Toledo, Ohio 43606, USA

V. I. Kozub
A. F. Ioffe Physico-Technical Institute, 196021 St. Petersburg, Russia

I. V. Karpov
Intel Corporation, RN3-01, 2200 Mission College Boulevard, Santa Clara, California 95052, USA

V. G. Karpov*
Department of Physics and Astronomy, University of Toledo, Toledo, Ohio 43606, USA

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We present a comprehensive theoretical study of $1/f$ noise in chalcogenide glasses aimed at applications to the developing technology of phase change memory. Our consideration is based on a body of formerly established facts about the atomic and electronic excitations specific to the chalcogenide glasses, which have not been considered in recent work; we give a brief survey of the relevant information. Our analysis reveals three possible mechanisms of $1/f$ noise in chalcogenide glasses: mobility fluctuations due to transitions in the double-well potentials of the glass, concentration fluctuations due to the same, and generation-recombination noise due to multiphonon electronic transitions in the quasicontinuous spectrum of electronic states in the mobility gap. We show that double-well potentials are the most likely source of the observed $1/f$ noise. Furthermore, we discriminate between the double-well potentials of atomic and electronic nature. The latter are related to the spatially close (intimate) pairs of oppositely charged negative-U centers and provide a much stronger effect on the $1/f$ noise. Our theory gives explicit expressions for the noise amplitude and the Hooge parameters corresponding to all mechanisms of $1/f$ noise in chalcogenide glasses. Most of these expressions are obtained in both a simplistic intuitive way and by means of much more involved rigorous analysis provided in the paper's Appendixes.

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I. INTRODUCTION

The recent developments in phase change memory (PCM) (Ref. 1) revived interest in the physics of chalcogenide glasses. We recall that PCM utilizes electrically initiated reversible amorphous-to-crystalline phase changes in multicomponent chalcogenide materials, such as $Ge_2Sb_2Te_5$ (GST); their markedly different phase resistances are used as the two logic states.

Not surprisingly, the new technology triggered a "rediscovery" of the underlying materials: understanding chalcogenide glasses became vitally important for PCM device engineering. To some degree, this rediscovery has overlooked a number of important concepts (see Sec. II below) concerning the physics of localized atomic and electronic states in glasses that had been previously established in the 1970s and 1980s. Instead, several concepts more relevant to classical crystalline materials (Si, Ge, and $A^{III}B^{IV}$) were postulated to hold true for chalcogenide glasses, including those of high hole mobility, donors and acceptors, hopping conduction, avalanche processes, etc.[2,3] Employing the highly developed physics of crystalline materials, rather than the earlier acquired understanding of glasses, made it convenient to extensively apply commercial software, developed for the crystalline device industry, in which the many fitting parameters enable one to tweak crystalline-based models to match practically any of the dependencies measured in PCM glasses.[4]

Here we analyze $1/f$ noise, which is a disorder related phenomenon whose features are very sensitive to the details of underlying physics. The experimental observations[5–9] show that in chalcogenides the $1/f$ noise power spectrum amplitude remains proportional to the square of dc current under low enough voltages while it becomes superlinear in dc current when the dc voltage and current increase toward their switching values. Such nonlinear $1/f$ noise was observed in other systems, of which the most similar is a-Si:H.[10]

Our approach here is based on considering all possible sources of $1/f$ noise consistent with the established properties of atomic and electronic localized states in chalcogenide glasses. It appears appropriate then to start with a brief survey of such properties, which we present in Sec. II below. In Sec. III we discuss specific atomic and electronic excitations capable of generating $1/f$ noise in chalcogenide glasses, and show how $1/f$ noise results from an exponentially broad spectrum of random relaxation times. Section IV gives semiquantitative estimates of the Hooge parameter corresponding to conceivable sources of $1/f$ noise in chalcogenide glasses. As the corresponding rigorous derivations turned out to be rather long, we chose to present them in Appendixes A–C of this paper. Conclusions are given in Sec. V.

II. SURVEY OF ATOMIC AND ELECTRONIC LOCALIZED STATES IN CHALCOGENIDE GLASSES

Most of the information about localized states (excitations) in glasses was acquired by 1980; the comprehensive

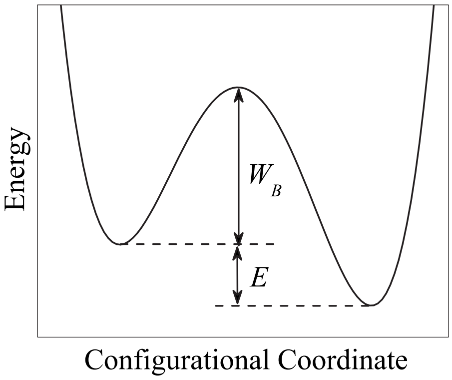

FIG. 1. Double-well atomic potential (DWP) with the barrier height W_B and difference between energy minima E. An atom can move between the minima causing fluctuations in atomic and electronic properties of the glass.

review by Mott and Davis[11] covers most of the electronic component with more limited reviews given later in Refs. 12 and 13. The atomic component was described in the reviews of Refs. 14–16 and applied to PCM in Ref. 17. Here, we briefly summarize the major concepts related to possible sources of noise.

A. Localized atomic excitations in glasses

Localized atomic states in glasses attracted a great deal of attention in connection with anomalous properties observed at low temperature (T), such as the specific heat $C \propto T$, thermal conduction $\chi \propto T^2$, absorption, and many others. These properties are now commonly understood based on the concept[18,19] of double-well potentials (DWP), according to which some atoms or small groups of atoms retain their mobility, even at very low T, by moving between two energy minima separated by a potential barrier W_B, as illustrated in Fig. 1. The potential barriers and the differences between the energy minima (asymmetry) E are described as random quantities that are almost uniformly distributed within their respective energy intervals, in particular $W_{B,\min} < W_B < W_{B,\max}$.

It is essential for our consideration that the DWP concept introduces the *exponentially broad distribution of relaxation times* $\tau(W_B) = \tau_0 \exp(W_B/kT)$. Because the barrier height W_B is a random quantity with almost uniform probabilistic distribution $g(W_B) \approx 1/\Delta W_B$, $\Delta W_B = W_{B,\max} - W_{B,\min}$ between its boundary values, the maximum and minimum relaxation times in the system are estimated as $\tau_{\max(\min)} = \tau_0 \exp(W_{B,\max(\min)}/kT)$. The relaxation-time distribution takes the form

$$\rho(\tau) = g(W_B)\left|\frac{dW_B}{d\tau}\right| = \frac{kT}{\tau \Delta W_B}, \quad \tau_{\min} < \tau < \tau_{\max}. \tag{1}$$

For relatively high temperatures, above tens of kelvins, the atomic tunneling phenomena in DWP can be neglected, in which case the joint probabilistic distribution of DWP parameters E and W_B takes the form

$$\rho(E,\tau) = \frac{kTP_T}{\tau \Delta W_B} \equiv \frac{P}{\tau}. \tag{2}$$

The parameters of the DWP distribution in glasses exhibit surprisingly modest variations between glasses of different chemical composition and are experimentally estimated as $P_T \sim 10^{20} - 10^{21}$ eV^{-1} cm^{-3} and $\Delta W_B \sim W_{B,\max} \sim 1$ eV; correspondingly, $P \sim 10^{18} - 10^{19}$ eV^{-1} cm^{-3}. The DWP relaxation-time interval $\tau_{\min} < \tau < \tau_{\max}$ is exponentially broad ranging from $\tau_{\min}$ comparable to the characteristic atomic vibration times $\tau_0 \sim 10^{-13}$ s to extremely long times $\tau_{\max}$ on the scale of months and years (at room T).

DWP interact with both the atomic and electronic systems of a glass. In particular, they can affect the scattering of charge carriers. Since the two different equilibrium configurations in a DWP have different scattering cross sections, random transitions in DWP will modulate the charge-carrier mobility. In addition, atomic transitions in DWP can modulate the electron energies through the deformation potential or electric-dipole interaction, causing fluctuations in the concentration of charge carriers above the mobility gap.

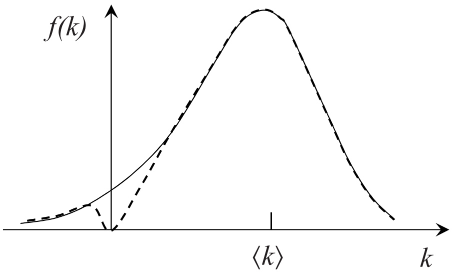

FIG. 2. Probabilistic distribution of local spring constants in a glass. The solid line shows the original distribution suggested in Ref. 20 while the dashed line accounts for the later established (Ref. 14) low-k singularity $f(k) \propto |k|$. Soft atomic potentials are characterized by $k \ll \langle k \rangle$.

Later work[14,20] extended the DWP model by assuming a continuous distribution (Fig. 2) of microscopic spring constants k in the anharmonic atomic potential

$$V(x) = kx^2/2 + Bx^3 + Cx^4,$$

where x is a generalized configuration coordinate of unspecified microscopic nature, and B and C are constant coefficients of expansion. The region of $k < 0$ represents DWP of relatively low concentration related to the decay of the distribution tail toward small and negative values. Furthermore, its rapid decay suggests that the majority of DWP are "soft" atomic potentials with $k \ll \langle k \rangle$, where $\langle k \rangle$ is the average spring constant close to the typical values in solids. Among the many verified phenomena related to soft atomic potentials,[14,21] here we emphasize their gigantic susceptibility $\propto 1/|k|$, implying an abnormally strong interaction with electrons.[22]

B. Localized electronic excitations in glasses

Experimental data on the various electronic properties of chalcogenide glasses can be broken into two groups, one of which testifies in favor of a high concentration of localized

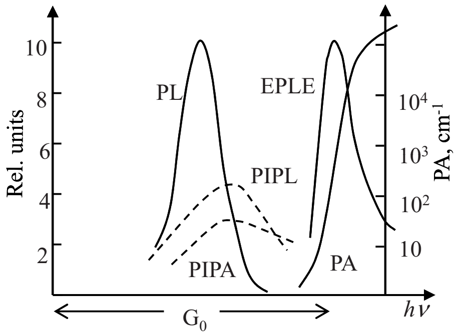

FIG. 3. Sketch of the typical spectroscopic data in chalcogenide glasses: photoabsorption (PA), photoluminescence (PL), efficiency of photoluminescence excitation (EPLE), photoinduced PL enhancement (PIPL), and photoinduced photoabsorption (PIPA) vs photon energy. All the curves except PA are plotted against the left vertical axis. G_0 is the optical gap.

states while another states the opposite. The latter group includes: lack of electron-spin-resonance (ESR) signal, absence of hopping conduction, optical gap G_0 approximately equal to the mobility gap G, and lack of absorption of photons of energy much lower than G. The former group, on the other hand, includes observations of strong photoinduced ESR corresponding to the electron concentration $\lesssim 10^{20}$ cm^{-3}, photoluminescence (PL) with energy close to $G/2$, dc screening length revealing the defect concentration of $\lesssim 10^{19}$ cm^{-3}, strong pinning of the Fermi level close to the midgap, photoinduced midgap absorption, and photoinduced change in the midgap photoluminescence. The spectroscopic aspects of these facts are illustrated in Fig. 3.

A solution to the above controversy was proposed by Anderson[23] who put forward the concept of negative-U (negative Hubbard or negative correlation) energy implying that two identical charge carriers localized at the same center will attract in spite of the Coulomb repulsion. As a result, double occupancy of a localized state becomes energetically more favorable than single occupancy of two localized states, such that the equilibrium occupation is $n=2$ (electrons or holes) while $n=1$ can only exist as an excited state. This obviously explains the lack of ESR in spite of high concentration of localized (doubly occupied) states in the vicinity of the Fermi level. Also, the photoinduced effects become attributable to the nonequilibrium single-occupancy states excited by higher energy photons.

The nature of negative-U energy is specified as being related to an abnormally strong electron-lattice interaction for localized charged carriers. The energy of $n=0,1,2$ localized carriers is described as

$$E_n(x) = nE_0 + kx^2/2 - nQx + U_c\delta_{n,2}, \tag{3}$$

where E_0 is the bare energy of the center, x is the lattice deformation around the center, Q is the deformation potential, and U_c is the Coulomb repulsion energy applicable when $n=2$. The dependencies in Eq. (3) are illustrated in Fig. 4.

The equilibrium energies are given by the equation

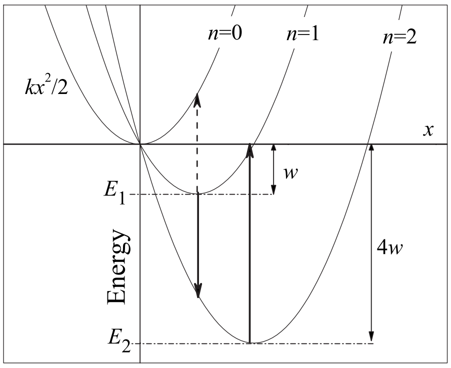

FIG. 4. Energies of n localized charge carriers vs the local lattice deformation x. The upward solid arrows represent absorption and the downward solid arrows represent photoluminescence processes. The dashed arrow indicates photoinduced photoabsorption from the nonequilibrium $n=1$ state. E_1 and E_2 represent the equilibrium energies for $n=1$ and $n=2$ localized carriers. w is the polaron shift and U_c is assumed to be relatively small.

$$E_n = nE_0 - n^2 w + U_c\delta_{n,2}, \quad \text{with} \quad w \equiv \frac{Q^2}{2k}, \tag{4}$$

where w is called the polaron shift. The correlation energy is given by

$$U \equiv E_2 - 2E_1 = -2w + U_c. \tag{5}$$

The negative U corresponds to a strong polaron effect with $w > U_c/2$.

By the Franck-Condon principle, the characteristic energy of the absorbed light in Fig. 4 is $|E_2|$ while that of emission (PL) and photoinduced absorption is $2|E_1|$, and, assuming U_c is relatively small, $|E_2| \approx 4|E_1|$, consistent with the data in Fig. 3. These transitions are shown in Fig. 5 with respect to the mobility gap. Comparing Figs. 3–5 enables one to estimate $w \approx G/4$ (although w can be somewhat different for the cases of electrons and holes[11]).

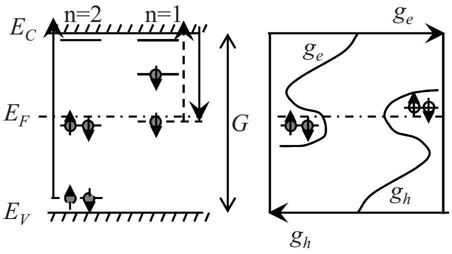

FIG. 5. Left: one-particle energy levels (i.e., energy per particle) corresponding to $n=2$ and $n=1$ electrons in the mobility gap. The levels without electrons represent the bare energy. Solid and dashed lines indicate thermodynamic and optical energy levels, respectively. The dashed electron level close to the valence-band edge represents the energy needed to optically ionize the $2e$ state (solid upward arrow); the solid level close to the midgap represents the energy needed to thermally ionize the same $2e$ state. The arrows have the same meaning as in Fig. 4. Right: density of the two-electron (g_e) and two-hole (g_h) states vs their one-particle energies where negative-U centers near the Fermi level provide its pinning.

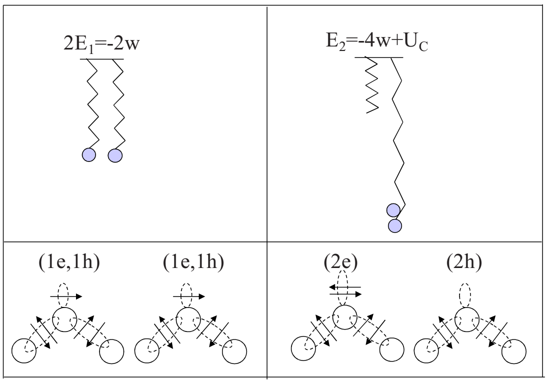

FIG. 6. (Color online) Mechanical analogy of the negative-U effect consisting of two elastic springs and two charged balls that can be attached to the springs either separately or together (top row), and its simple model based on the valence bonds representation (bottom row) where two electrons can occupy the states of two broken bonds or one dangling bond. The right column is energetically more favorable when $w > U_c/2$.

Drawing similar energy levels for holes and allowing for some dispersion leads to the right diagram in Fig. 5 that explains how the Fermi level is pinned by a high concentration of $2e$ and $2h$ states forming a gapless spectrum of two-particle excitations. In addition to the pinning $(2e,2h)$ states, shown in the same diagram are band tails possessing the characteristic decay scales on the order of several hundredths of eV. They can contribute to optical absorption and act as shallow traps underlying dispersive transport and other phenomena.[12] As shown in Fig. 5, the one-particle excited states $1e$ and $1h$ are obtained through the partial ionization of $(2e,2h)$. Possessing energies of approximately $w = G/4$ from the corresponding mobility edges, they can affect transport phenomena.[13]

The microscopic nature of negative-U centers is not particularly important for the purposes of this work; here we limit ourselves to a brief comment on the subject. We note that the negative-U phenomenon can be simply illustrated in terms of a mechanical analogy with two electrically charged balls, each of weight Q, which can be attached to either two different elastic springs or one such spring, as depicted in Fig. 6.

Street and Mott[24] proposed a microscopic model where $2e$ and $2h$ states correspond to certain defect states (D^- and D^+) while $1e$ and $1h$ are the same dangling bond (D^0). Kastner and co-workers[25] introduced more specific consideration taking into account the chemical nature of chalcogenide forming atoms; in their popular notation D^- and D^+ are represented as C^{1-} and C^{3+} where the superscript indices refer to defect coordination numbers.

Later work[22] emphasized that a theoretical description of the negative U must explain the observed significant polaron shift w. The required shift was attributed to centers with abnormally small spring constants k (soft atomic potentials) that exist in glasses due to their inherent structural disorder, as was discussed in connection with Fig. 2. In particular, the polaron shift $w \approx G/4$ implies the spring constant $k_G \approx \langle k \rangle (2\langle w \rangle / G) \ll \langle k \rangle$, where $\langle w \rangle \lesssim 0.1$ eV is the average polaron shift corresponding to the average spring constant $\langle k \rangle$ which describes the macroscopic properties of glasses.

It should be remembered that the $2e$ and $2h$ gapless excitations typically have extremely long relaxation times related to the necessity of carrying a heavy polaron cloud (i.e., atomic deformation) in the course of electron transitions. Here we will describe such slow transitions in terms of electronic DWP with a transition barrier W_B related to the polaron shift. The two minima of such a DWP will correspond to the charge states (0,0) and $(2e,2h)$ of two centers with energies close to the Fermi level.

The transition barrier $W_B \approx 8w \approx 2G$ (first estimated by Phillips[26]) is high enough to fully suppress dc hopping conduction that could occur through electron hopping between centers separated by distances of the order of the average intercenter distance.[11] Assuming, for specificity, $2G \approx 1.6$ eV for the case of GST glasses and implementing the standard estimates[11] yields the multiplier $\exp(-2G/kT) \sim 10^{-27}$ in the electron transition rate. This predicts hopping conduction many orders of magnitude below what is observed both in the nonglassy semiconductors (such as a-Si) and the band conduction in chalcogenide glasses [small by the factor $\exp(-G/kT)$ instead of $\exp(-2G/kT)$ for hopping].

In the latter estimate, we have neglected both the quantum contribution caused by the overlap of the wave functions of spatially close $2e$ and $2h$ centers, and the Coulomb interaction of $2e$ and $2h$ pairs. It was shown[27] that both corrections are significant for the case of *spatially close* pairs, sometimes called intimate pairs, which can decrease the barrier height by several times. In particular, the intimate $(2e,2h)$ pairs partially decrease their energy due to the strong Coulomb interaction, which relaxes the requirement of very soft atomic potentials with $k \approx k_G$. Because higher k values result in smaller w, the factor $\exp(-8w/kT)$ describing the suppressing effect of a polaron cloud on the electronic transition becomes less significant, allowing for much higher hopping probabilities.

Lacking more accurate information, one can resort to the data[28] on alternating current (ac) conduction in chalcogenide glasses that is comparable to that of other noncrystalline semiconductors at low frequencies and strongly decays at higher frequencies. Because ac conduction is attributed to electron hopping between close centers,[28] these observations can be explained[27] by significant suppression of the transition barrier for intimate pairs.

The activation relaxation time for the electronic DWP can be estimated as

$$\tau = \tau_{\min} \exp\left[\frac{2R}{a} + \frac{\Delta W_B(R)}{kT}\right], \tag{6}$$

with $\tau_{\min} = \tau_0 \exp[W_B(R_{\min})/(kT)]$ and $\Delta W_B = W_B(R) - W_B(R_{\min})$, $(\Delta W_B)_{\max} \approx 2G$, where R is the intercenter distance, a is the electron localization radius at the center, $\exp(2R/a)$ describes the electron tunneling, and $W_B(R_{\min})$ is the activation barrier for intimate pairs separated by the distance $R_{\min} \sim a$. Because R is a random quantity with the probabilistic distribution $4\pi R^2 N_U$, where N_U is the concentration of negative-U centers, the probabilistic distribution of relaxation times becomes qualitatively similar to that in Eq. (2),

$$\rho(E,\tau)=\frac{P}{\tau},\quad P\approx\frac{\pi N_U^2 a^3}{4\Delta E_U}\frac{[\ln(\tau/\tau_{\min})]^2}{1+G/kT},\tag{7}$$

where we have used a rough estimate $dW_B/dR \sim (\Delta W_B)_{\max}/a$ and where ΔE_U is the total-energy width of the negative-U center distributions that are approximately uniform in the proximity of the Fermi level. In what follows we neglect the logarithmically weak dependence of P vs τ and treat it as a constant.

One outstanding feature of electronic DWP is the gigantic dipole moment $p=2eR$ that for the typical $R=N_U^{-1/3}$ is many orders of magnitude higher than that of the atomic DWP discussed earlier. As a result, electronic DWP are expected to be a much stronger noise source.

For numerical estimates we use the values discussed in Sec. IXD of Ref. 11 that suggest $N_U\sim 10^{17}-10^{18}$ cm^{-3} and $\Delta E_U\sim 0.025$ eV, yielding $P\sim 10^{15}-10^{17}$ eV^{-1} cm^{-3}, which is lower than that of the atomic DWP. The transition time τ corresponding to the typical $a\sim 10$ Å, average $R\sim N_U^{-1/3}$, and $W_B\approx 2G\sim 2$ eV turns out to be long enough to fully suppress hopping conduction.[26] On the other hand, as mentioned above, spatially close (intimate) pairs can have much lower W_B and exponentially shorter relaxation time than distant pairs, thus making noticeable contributions to the system noise in a broad range of relatively low frequencies.

We shall end this section with a conclusion of the existence of both atomic and electronic localized states described in terms of atomic and electronic DWPs that have exponentially broad distributions of relaxation times covering the low-frequency interval typical of 1/*f* noise measurements. These distributions are generally proportional to $1/\tau$, which is known[29,30] to lead to the 1/*f* power spectrum of fluctuations (see below).

III. POSSIBLE SOURCES OF 1/f NOISE IN CHALCOGENIDE GLASSES

1/*f* noise in the electric current, also known as excess noise, is due to resistance fluctuations. Indeed, the measured mean-square-root current fluctuation δI related to 1/*f* noise is proportional to the current I itself, in contrast to, e.g., the equilibrium Nyquist noise. It is generally attributed to independent microscopic degrees of freedom ("fluctuators") possessing exponentially broad distributions of relaxation times that affect the material resistance. That general understanding originally suggested in Ref. 31 was later specified for a mechanism related to surface traps in semiconductors[32] (later supranationally generalized[33]). A possible contribution to the noise from structural two-level systems related to DWP (Refs. 18 and 19) was first discussed in Refs. 34 and 35.

As explained in Sec. II above, another class of fluctuators in glasses can be related to DWP of electronic nature formed by $(2e,2h)$ pairs of charged carriers. We note that 1/*f* noise due to general intercenter hopping[36] was studied in Ref. 37. However, it was pointed out[38] that in typical hopping insulators the characteristic relaxation times for such pairs have a relatively low upper limit due to the fact that pairs separated by distances longer than the average are exponentially unlikely; hence, hopping conduction can hardly be a general source of 1/*f* noise [$(2e,2h)$ pairs are an exception owing to their extremely long hopping times due to the strong polaron effect underlying the negative-U phenomenon].

The concept of "aggregates" formed by a set of pairs of centers (or "quasispins") was suggested[39] to explain the observed absence of the frequency cutoff of 1/*f* noise in hopping conductivity. These aggregates with strong Coulomb correlations were shown to have at least two metastable configurations that differed by the distribution of electron charges. The transitions between them are of multielectron nature with relaxation times that exponentially increase with the number of electron sites involved. We note however that the concept of aggregates is limited to the relatively low-temperature regime, $kT\ll\Delta_C=[g(E_F)e^6/\kappa^3]^{1/2}$, where Δ_C is the Coulomb gap,[39] and κ is the dielectric permittivity. Given the typical $g(E_F)\lesssim 10^{18}$ cm^{-3} eV^{-1} and $\kappa\sim 10$, the opposite inequality holds for chalcogenide glasses at room temperature. As a result, the $(2e,2h)$ pairs described in Sec. II remain the only candidate electronic two-state systems in chalcogenide glasses.

Since the extensive work of 1960–1980, it has become common understanding[11] that dc conduction of chalcogenide glasses is due to the charge carriers excited above the mobility edge, at least for temperatures that are not too low ($T \gtrsim 100$ K), and in particular at room temperature. The noise in the corresponding conductivity $\sigma=ne\mu$ can be due to fluctuations in carrier concentration n and mobility μ which are attributable to fluctuations in some internal degrees of freedom.

Following the standard approach, we assume that each frequency component of the noise is related to the corresponding partial source of fluctuations characterized by its relaxation time $\tau=1/f$ and that there exists a very broad distribution of τ. The shape of such a distribution $\rho(\tau)$ deduced from the noise spectrum $f(\omega)\propto 1/\omega$ becomes

$$\rho(\tau)=\left|\frac{d\omega}{d\tau}\right|f(\omega=1/\tau)\propto\frac{1}{\tau}.\tag{8}$$

We observe that the distributions in Eqs. (1) and (7) fit the requirement of Eq. (8) quite nicely.

The latter observation has a well-known generalization: the relaxation-time distribution $\rho\propto 1/\tau$ appears when τ is an exponential function of some uniformly distributed random parameter λ:

$$\rho(\tau)=\left|\frac{d\lambda}{d\tau}\right|\text{const}\propto\frac{1}{\tau},\tag{9}$$

where we have taken into account that $\lambda=\ln(\tau)$. In particular, λ is represented by the random quantities W_B/kT and $2R/a$ for the cases of atomic and electronic DWPs in Eqs. (1) and (7), respectively.

One other conceivable representation of λ is related to generation-recombination noise where $\lambda=E/kT$ with E being energy in a quasicontinuous spectrum of localized states in the mobility gap.[40,41] In that case, the fluctuations in free-carrier concentration are due to variations in the occupation numbers of localized states whose relaxation times $\tau \propto \exp(E/kT)$ are determined by trapping and detrapping of

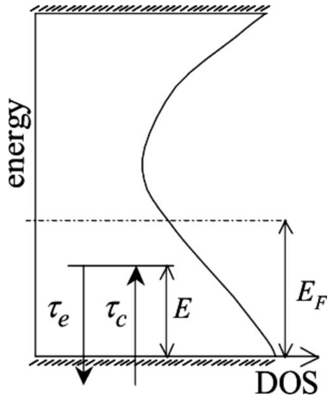

FIG. 7. Sketch of the density of localized states in the mobility gap of a noncrystalline semiconductor and processes of the electron capture to and emission from the level of energy E. E_F is the Fermi energy.

charge carriers. These relaxation times can be long enough to correspond to $\tau^{-1}=\omega$ in the low-frequency region of the $1/f$ noise observations.

At the first glance, the relation $\rho(\tau)\propto 1/\tau$ takes place when the density of states (DOS) is uniform, $g(E)=\text{const}$, and it approximately holds true for a nonuniform $g(E)$ (of the kind depicted in Figs. 5 and 7) provided that its characteristic energy scale E_0 is considerably greater than kT. However, the partial contributions of states with different energies E are determined by their occupation numbers $n_E\propto \exp(E/kT)$ (in the region far from the Fermi level that is significant at frequencies that are not too low). As a result, one gets $g(E)\propto \exp(E/kT)$ for the density of *effective* (i.e., contributing) states. This entails

$$\rho(\tau) = g[E(\tau)]\left|\frac{dE}{d\tau}\right| = \text{const} \quad \text{and} \quad f(\omega)\propto \frac{1}{\omega^2}, \qquad (10)$$

consistent with the result of the derivation in Ref. 41. Furthermore, at very low frequencies, the noise is determined by the slowest active localized states that belong to the energy band of width $\sim kT$ around the Fermi level and behave effectively as a single energy level. Applying the known result for generation-recombination noise due to discrete levels[29,30] predicts frequency-independent noise.

Assuming a strongly varying DOS, often modeled with an exponential shape,[40,41] $g(E)\propto \exp(-E/E_0)$, with $E_0=\text{const}$, does not change the latter observation considerably: the generation-recombination mechanism in the bulk (also known as bulk trapping/detrapping) is generally inconsistent with the $1/f$ noise spectrum. (We note that, however, interface related trapping/detrapping can be significant[32,33] but that topic is beyond our present scope.) The possibility of bulk trapping/detrapping related $1/f$ spectrum arises again[40,41] if the charge-carrier trapping time exponentially increases with E [i.e., $\tau_c\propto \exp(E/\varepsilon)$] due to the multiphonon nature of trapping processes where $\varepsilon\sim 0.01-0.03$ eV is of the order of the characteristic phonon energy.[11,42,43] It was shown indeed[44] that such multiphonon processes can be responsible for a variety of observed phenomena in noncrystalline semiconductors. In the case of strong energy dependence, $\varepsilon \ll kT$ and $\varepsilon \ll E_0$, the energy dependencies of occupation numbers and density of effective states become insignificant, which restores the $1/f$ noise spectrum.

We believe that the mechanisms discussed in this section cover all possible sources of bulk $1/f$ noise in chalcogenide glasses; they are: mobility and concentration fluctuations due to transitions in the atomic and electronic double-well potentials, and fluctuations in carrier concentration due to generation-recombination multiphonon processes in the quasicontinuous electronic spectrum.

In contrast to the latter statement, two papers[5,6] studying $1/f$ noise in chalcogenide switches and PCM devices speculated that it could be due to avalanchelike multiplication processes. That hypothesis is inconsistent with the common knowledge that avalanche processes generate white noise (and even serve as white-noise generators),[45] and that a concomitant $1/f$ component (if observed) is not directly related to the current flowing under avalanche breakdown conditions.[46] Reference 6 attributed an observed $1/f$ component to avalanche processes simply based on the assumption that such processes are responsible for the observed switching. The authors of Ref. 5, while recognizing the contradiction with the established white spectrum, referred to the fact that a $1/f$ noise component had been observed in some avalanche based devices. We note that the simultaneous observation of two phenomena does not generally prove that they are in cause and effect relation with each other.

Finally, we note that our analysis is limited to the linear regime in which, "…the current passing through the material is simply a probe of, and does not cause, the electronic noise."[10] In spite of this limitation, we shall see in what follows (Table I) that some of our analyzed noise mechanisms predict the noise amplitude to be a function of carrier concentration n_c, which is known to depend on voltage (or current) in chalcogenide glasses. As a result, even though the mechanisms are linear in nature some of our predictions will resemble nonlinear behavior, for example, $\Delta j^2\propto n_c j^2\propto j^3$, where j is the electric current density and Δj its dispersion. This kind of "inexplicit" nonlinearity should be differentiated from models in which the current directly influences the noise, such as that of Ref. 10 or work regarding non-Ohmic structures (devices).[45,47,48]

IV. QUANTITATIVE ESTIMATES OF 1/*f* NOISE IN CHALCOGENIDE GLASSES

The standard quantitative metric of noise characterization is $(\Delta j)^2/j^2$, where the numerator represents the electric current-density dispersion and j is the average amplitude of the direct current density. In the frequency representation, $(\Delta j)^2$ is measured per unit frequency band making it independent of the measuring device frequency band $\Delta\omega$; hence, the ratio $(\Delta j)^2/j^2$ has the dimension of reciprocal frequency. The corresponding dimensionless metric, called the Hooge parameter,[47] is defined as

$$\alpha = \frac{\Delta j^2}{j^2}\frac{\omega N_e}{2\pi}. \qquad (11)$$

Physically, the Hooge parameter is the noise amplitude per charge carrier corresponding to the frequency band equal to

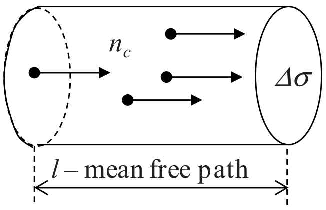

FIG. 8. Sketch of the quasiclassical $1/f$ noise mechanism of electron (hole) mobility modulation by fluctuations of the electron (hole) scattering cross section $\Delta\sigma$ due to DWP related scatters. Arrows represent the drift velocities of the charge carriers of concentration n_c.

the frequency per se, $f=\omega/2\pi$. It is understood that the direct current square is proportional to N_e^2 while the current dispersion is proportional to the total number $N_e \gg 1$ of charge carriers, whose contributions are statistically independent. Experimentally estimated Hooge parameters for different systems range from 10^{-9} to 10.

The concept of the Hooge parameter has known limitations.[49] In particular, the original suggestion that it is independent of charge-carrier concentration has been disproved many times (including in the results of the present work). However, we have chosen to keep it here because it is a commonly known dimensionless metric of $1/f$ noise that is often used in the representation of experimental results.

In this section we derive quantitative estimates of the Hooge parameter for all the conceivable cases of $1/f$ noise listed in Sec. III above. Here we employ certain approximations that make our consideration physically transparent and concise. The corresponding rigorous derivations leading to the same results are provided in Appendixes A–C.

A. Double-well potentials: mobility modulation mechanism

We conjecture that some fraction of the scattering centers are DWP which can have two possible scattering cross sections, different on average by $\Delta\sigma$, depending on the position of the atom at the time of scattering. This fluctuation in cross sections results in a concomitant change in charge-carrier mobility. As illustrated in Fig. 8, a cross-section change in just one scatterer will correspondingly change the number of scattering events ΔN_e, which results in the current-density fluctuation

$$\Delta j_1 = j\frac{\Delta N_e}{N_e} = j\frac{l\Delta\sigma n_c}{N_e},$$

where we have employed the standard quasiclassical picture based on the mean-free-path concept with l representing the mean-free path and n_c the charge-carrier concentration. The corresponding dispersion is obtained through multiplication by the total number ΔN_{DWP} of DWP belonging to the frequency band $\Delta\omega$ of transition rates,

$$(\Delta j)^2 = j^2\frac{(l\Delta\sigma)^2 n_c^2}{N_e^2}\Delta N_{\mathrm{DWP}}.$$

Based on the distribution functions in Eqs. (2) and (7), and taking into account that $\Delta\omega/\omega=\Delta\tau/\tau$ the latter number becomes

$$\Delta N_{\mathrm{DWP}} = PkTV\frac{\Delta\omega}{\omega}. \tag{12}$$

Substituting the above estimates into the definition of Eq. (11) finally yields

$$\alpha = \frac{(l\Delta\sigma)^2 n_c PkT}{2\pi}, \tag{13}$$

where we have introduced the electron (hole) concentration $n_c=N_e/V$. This result differs from that of the rigorous consideration in Eq. (A33) by a numerical multiplier of order unity.

Consider first numerical estimates for the case of atomic DWP. Assuming the geometrical cross section of the characteristic atomic dimension, we put $\sigma \sim 10^{-16}$ cm^2 and $\Delta\sigma \sim 10^{-17}$ cm^2 for its relatively small change. Also, we assume the typical $l \sim 100$ Å, room temperature $kT=0.025$ eV, and the electron concentration $n_c \sim 10^{16}$ cm^{-3}. Using then $P \sim 10^{18}$–10^{19} eV^{-1} cm^{-3} [see the discussion after Eq. (2)] yields $\alpha \sim 10^{-14}$–10^{-13}, significantly lower than the experimentally estimated Hooge parameter values.[30]

On the other hand, the case of electron DWP, predicts a much greater Hooge parameter due to a considerably stronger scattering effect by the $(2e,2h)$ pair dipole. In that case

$$\Delta\sigma = \sigma \sim \frac{\pi p}{kT\kappa},$$

where κ is the dielectric permittivity and we used the standard quasiclassical estimate for the dipole interaction radius: $pe/(\kappa r^2)=kT$. As a rough estimate let $p=(1$–$3)\times 2ae$ [implying intercenter distances of $(1$–$3)a$] and $\kappa \sim 10$ which yields $\sigma \sim 10^{-11}$–10^{-12} cm^2. Combining this with the above estimated $P \sim 10^{17}$–10^{18} eV^{-1} cm^{-3} yields $\alpha \sim 10^{-5}$–10^{-2}, which is in the range of expected values.

A comment is in order regarding the above numerical estimate with $l \sim 100$ Å. That value was chosen to be a lower bound of the mean-free path consistent with the Ioffe-Regel criterion of extended (nonlocalized) states: $l \gtrsim \lambda$ where the DeBroglie wavelength for the charge carriers is $\lambda \sim \hbar/\sqrt{m^* kT} \sim 100$ Å and m^* is the effective mass. If experimental data indicates that l falls below λ (as often happens), then the mechanism of conduction may be more complex than simple band transport. We note that, however, even if we assume $l=10$ Å, our estimate for the electronic DWP $(\alpha \sim 10^{-7}$–$10^{-4})$ still remains in the ballpark of experimentally observed values.

B. Double-well potentials: concentration modulation mechanism

Atomic transitions in the double-well potentials of chalcogenide glasses can affect the electron energy levels causing changes in their occupation numbers, thereby modulating the charge-carrier concentration. Referring to Appendix B for a more rigorous treatment, here we give a semiquantitative estimate of that effect for the cases of small and large electron energy modulation amplitudes.

1. Small modulation amplitude

Consider first the case of relatively small amplitude modulation of the electron energy levels, $\delta E \ll kT$. We start with noting that changes in occupation of localized states near the Fermi level $\delta f \approx (\delta E/kT)f$ dominate the free-carrier-concentration modulation. The number of such centers is estimated as $N_T = g(E_F)kTV$, where $g(E_F)$ is the density of states at the Fermi level. We assume that each of those states with $f \sim 1/2$ changes its occupation number by $\delta f = (D/kT)\delta n_{\mathrm{DWP}}$, where D is the interaction energy of a DWP and a localized electron, and δn_{DWP} (of order unity) is the change in the DWP occupation number. As a result the change in the number of free charge carriers per center can be estimated as

$$\delta N_{e1} = \frac{D}{kT}\delta n_{\mathrm{DWP}} \exp\left(-\frac{E_F}{kT}\right),$$

where the exponential translates the effect at the Fermi energy states to the mobility edge. To estimate the corresponding dispersion in the frequency interval $\Delta\omega$, we multiply δN_{e1}^2 by the number of DWP ΔN_{DWP} in the volume a^3 of the localized state and the number N_T of such states where ΔN_{DWP} is given in Eq. (12), which yields

$$(\Delta N_e)^2 = D^2 P a^3 g(E_F) V \exp\left(-\frac{E_F}{kT}\right)\frac{\Delta\omega}{\omega}.$$

To obtain the relative current dispersion we divide the latter quantity by the square of the average carrier number $VN_{\mathrm{eff}}\exp(-E_F/kT)$, where N_{eff} is the effective density of states at the mobility edge. As a result we get

$$\frac{(\Delta j)^2}{j^2} = D^2 P a^3 g(E_F)\frac{\Delta\omega}{\omega V N_{\mathrm{eff}}^2},$$

and the corresponding Hooge parameter

$$\alpha = \frac{D^2 P a^3 g(E_F) n_c}{2\pi N_{\mathrm{eff}}^2}. \qquad (14)$$

This result coincides with that of Appendix B to the accuracy of an insignificant numerical factor.

For numerical estimates we assume $D \sim 1$ eV corresponding to the electronic DWP, $a \sim 10$ Å, $n_c \sim 10^{16}$ cm^{-3}, $N_{\mathrm{eff}} \sim 10^{18}$ cm^{-3}, $g(E_F) \sim 10^{17}-10^{18}$ cm^{-3} eV^{-1}, and $P \sim 10^{17}-10^{18}$ cm^{-3} eV^{-1}, which gives $\alpha \sim 10^{-7}-10^{-6}$, in the range of known values yet considerably lower than the mobility modulated noise.

On the other hand, for atomic DWP, the estimate in Eq. (14) will contain an additional small multiplier reflecting the smallness of the atomic DWP dipole moment. This decreases α below the range of practical interest; hence, atomic DWP do not make any significant contribution in either the mobility or concentration modulation mechanisms of $1/f$ noise.

2. Large modulation amplitude

Consider next the opposite limiting case of very large modulation amplitude $\delta E \sim E_F \gg kT$, which may be possible when the electron trap is situated in the nearest proximity of the electronic DWP. The interaction energy $U = 2e^2/\kappa r$ between the trap and the $2e$ (or $2h$) part of the electronic DWP is so large that the DWP and the trap cannot be considered separately but rather as an aggregate in which DWP transitions are strongly coupled with trapping/detrapping processes. The trap energy is supposed to fall in the nearest proximity of the Fermi level so that the number of suitable traps is given by the same equation as the above, $N_T = g(E_F)kTV$.

To make the aggregate excitation energy low enough ($\lesssim kT$), we assume that the DWP asymmetry is within the interval of kT from the trap energy $E \approx E_F$. Two energy states of such an aggregate will then correspond to the following combinations: (1) filled trap+higher energy DWP state, and (2) empty trap+lower energy DWP state. The number of suitable DWP per trap is estimated as

$$\Delta N_{\mathrm{DWP}} = PkT\frac{\Delta\omega}{\omega}\left(\frac{2e^2}{E_F\kappa}\right)^3.$$

Dividing the product $N_{\mathrm{DWP}}N_T$ by the square of the number of free carriers Vn_c gives the relative dispersion of both the free-carrier concentration and the current. The corresponding Hooge parameter becomes

$$\alpha = \frac{g(E_F)P(kT)^2}{n_c}\left(\frac{2e^2}{E_F\kappa}\right)^3. \qquad (15)$$

Using the above numerical parameters, the aggregate related Hooge parameter can be comparable with the above estimated α due to the mobility modulated mechanism. A significant difference between the two results is that Eq. (15) predicts a decreasing Hooge parameter with increasing charge-carrier concentration while Eq. (13) states the opposite. Furthermore, the corresponding temperature dependencies are exponentially different and that may be used for experimental verifications. Also, the non-Ohmic behavior turns out to be very different: $(\Delta j)^2/j^2$ is expected to increase or decrease with increasing current in the non-Ohmic regime for the cases of Eq. (13) and (15), respectively.

C. Generation-recombination noise

We start with the general equation derived in Appendix C and describe generation-recombination noise for the case of a continuous energy spectrum of electronic states in the mobility gap,

$$\frac{\langle(\delta I)^2\rangle}{I^2} = \frac{4}{n_c^2 V}\int_0^\infty \frac{\tau^2 g(E)dE}{(\tau_e+\tau_c)(1+\omega^2\tau^2)}, \qquad (16)$$

where all the time parameters in the integrand are understood to be functions of energy and the parameters are defined in Appendix C. Here τ_e and τ_c stand for the times of escape and capture, and $\tau = (\tau_e^{-1}+\tau_c^{-1})^{-1}$. To the accuracy of model notation, the result in Eq. (16) was derived in Ref. 41 in connection with the noise attributed to band tails of doped crystalline semiconductors.

1. Field effect

Because the data on $1/f$ noise in chalcogenide glasses extends to the region of non-Ohmic conduction and correspondingly strong electric fields, our consideration below will be adjusted to account for the field induced effects. To describe the case of strong electric field $\mathcal{E}$ we phenomenologically introduce the enhancement factor $\phi(\mathcal{E})$ which acts to increase the emission rate $\gamma_e \rightarrow \gamma_e \phi(\mathcal{E})$. The underlying mechanism will remove charge carriers from discrete energy levels to the extended states thereby increasing the carrier concentration, $n_c \rightarrow n_c(\mathcal{E})$. Here we use a simple approximation

$$\frac{n_c(\mathcal{E})}{n_c(0)} = \phi(\mathcal{E}), \tag{17}$$

neglecting possible effects of the electric field on the capture coefficient γ_c and assuming a slowly varying density of states $g(E)$ in the proximity of the Fermi level. We note that the field function $\phi(\mathcal{E})$ can be exponentially strong. For example, the hole emission from negatively charged centers is described by the Pool-Frenkel[50] expression with

$$\phi(\mathcal{E}) = \exp(\sqrt{\mathcal{E}/\mathcal{E}_{\rm PF}}), \quad \mathcal{E}_{\rm PF} = (kT)^2 \kappa / e^3,$$

where κ is the dielectric permittivity. According to other publications, the exponent in $\phi(\mathcal{E})$ is linear in $\mathcal{E}$ (see references in Ref. 11). Here we maintain $\phi(\mathcal{E})$ as an experimentally known parameter related to the carrier concentration according to Eq. (17).

It follows from the above that in the presence of the electric field the emission and capture time parameters are related as

$$\frac{\tau_e}{\tau_c} = \frac{n_c \gamma_c}{N_{\rm eff} \gamma_e \phi} = \exp\left(\frac{E - E_F^*}{kT}\right), \tag{18}$$

where the quasi-Fermi level is given by

$$E_F^* = E_F + kT \ln[\phi(\mathcal{E})]. \tag{19}$$

2. Multiphonon transitions

A detailed discussion of multiphonon electronic transitions is found in Refs. 11, 42, and 43. Here we limit ourselves to noting that the dimensionless probability of simultaneously emitting N phonons in the process of capturing a charge carrier at a defect state with energy E in the mobility gap can be estimated as

$$\begin{aligned} p_N = p_1^N &= \exp[-N \ln(1/p_1)] \\ &= \exp[(-E/\hbar\omega_{\rm ph}) \ln(1/p_1)] \equiv \exp(E/\varepsilon), \end{aligned} \tag{20}$$

where $\hbar\omega_{\rm ph}$ is the characteristic phonon energy (of the order of the Debye energy). The energy parameter ε is typically in the range of 0.01–0.03 eV. Correspondingly, the time constant for the capture by an empty level can be written in the form

$$\tau_c = \tau_{c0} \exp(E/\varepsilon), \tag{21}$$

where $\tau_{c0} = 1/n\sigma v$ and σ is a hypothetical cross section of capture without the bottleneck of energy exchange. For the often assumed geometrical cross section $\sigma \sim 10^{-16}$ cm^2 and $n \sim 10^{16}$ cm^{-3}, one can estimate $\tau_{c0} \sim 10^{-7}$ s. The reverse process of emission from a filled level can be strongly facilitated by the external electric field.

3. Density-of-states model and evaluation of generation-recombination noise

Following Ref. 41, we assume a simple density-of-states model

$$g(E) = g_0 \exp(-E/E_0). \tag{22}$$

The characteristic values of E_0 (estimated, e.g., from the Urbach slope) are typically in the range of 0.03–0.1 eV, varying between different amorphous semiconductors.[51]

Based on Eqs. (C3), (16), and (18), the result in Eq. (16) can be presented in the form

$$\frac{\langle(\delta I)^2\rangle}{I^2} \approx \frac{4}{\omega (n_c \phi)^2 V} \int_0^\infty \frac{(\omega\tau) f(1-f)}{1+(\omega\tau)^2} g dE, \tag{23}$$

where f is the Fermi distribution. We then discriminate between two conceivable cases, which are different by the condition that the integral in Eq. (23) is determined by a narrow region close to the Fermi level where $f \approx 0.5$ or, alternatively, the region of $f \ll 1$ far from the Fermi level.

The former case occurs when kT is the smallest energy scale, $kT \ll E_0, \varepsilon$. For that case, Eq. (23) yields the result

$$\frac{\langle(\delta I)^2\rangle}{I^2} \approx \frac{1}{(n_c\phi)^2 V} g(E_F) kT \frac{\tau_F}{1+(\omega\tau_F)^2}, \tag{24}$$

with

$$\tau_F = (1/2) \tau_{c0} \exp(E_F^*/\varepsilon), \tag{25}$$

which never reduces to the $1/f$ noise.

For the latter case, one can approximate $f = \exp[-|E - E_F|/kT]$ and switch to integration over a new variable $z = \omega\tau$. Assuming $\omega\tau_{c0} \ll 1$ and $\omega\tau_F \gg 1$ evaluation of that integral yields

$$\frac{\langle(\delta I)^2\rangle}{I^2} \approx \frac{4 g_0 kT \varepsilon}{(n_c\phi)^2 V \tau_F^{\nu-1} E_0} \frac{1}{\omega^\nu}, \tag{26}$$

where

$$\nu = 1 - \frac{\varepsilon}{E_0} - \frac{\varepsilon}{kT}.$$

The result in Eq. (26) coincides with that of Ref. 41 to the accuracy of trivial modification $E_F \rightarrow E_F^*$ and a multiplier ϕ describing possible effects of non-Ohmicity. It reduces to the $1/f$ type of spectrum when $\varepsilon \ll kT, E_0$, in which case the Hooge parameter becomes

$$\alpha \approx \frac{2N_{\rm eff}}{\pi n_c \phi} \frac{\varepsilon}{kT} \exp\left(-\frac{E_F}{E_0}\right), \tag{27}$$

where we have taken into account that $N_{\rm eff} \approx g_o kT$. Assuming realistic $N_{\rm eff}/n_c \sim 100$, $\varepsilon/kT \sim 0.3$ and $\exp(E/E_0) \sim 10^{-6}$ gives $\alpha \sim 10^{-4}$, in the ballpark of the observed values.

We note that, however, the very possibility of $1/f$ noise here is contingent upon the rather strong assumptions of the inequalities $\omega\tau_{c0} \ll 1$, $\omega\tau_F \gg 1$, and $\varepsilon \ll kT, E_0$ that may not be quite general. For example, the parameters ε, kT, E_0 are comparable to each other for typical semiconductors and, therefore, the noise spectrum is far from the $1/f$ dependence. Given such degree of uncertainty, it is important to verify the voltage and current dependencies in Eqs. (26) and (27). Their distinctive feature is that both the relative dispersion $\langle(\delta I)^2\rangle/I^2$ and the Hooge parameter are predicted to decrease with I in the non-Ohmic region [as opposed to that due to DWP above]. Indeed, assuming standard transport at the mobility edge, the dc current $I\propto n_c\phi$ appears in the denominators of Eqs. (26) and (27). Not observing such a decrease in the noise amplitude with increasing current would rule out the generation-recombination mechanism as a possible source of $1/f$ noise.

V. CONCLUSIONS

We have presented and quantitatively described several conceivable mechanisms of bulk $1/f$ noise in chalcogenide glasses. All of them are related to the presence of random internal degrees of freedom (elemental fluctuators) with exponentially broad distributions of relaxation times, consistent with the existing general understanding of $1/f$ noise. We have related the physical origin of possible fluctuators to the established picture of localized atomic and electronic excitations in chalcogenide glasses. Such fluctuators were attributed to two-state microscopic systems of either atomic [double-well potentials (DWP)] or electronic nature (pairs of $2e$ and $2h$ negative U centers called electronic DWP throughout the paper), or strongly coupled aggregates of the latter with the deep electronic traps in the mobility gap. In addition, we have defined the conditions under which generation-recombination processes in the continuous electronic spectrum in the mobility gap can lead to $1/f$ noise. The analytical expressions and numerical estimates for the Hooge parameters for each mechanism are summarized in Table I. Our more specific conclusions are as follows.

(1) Atomic DWP that are responsible for low-temperature properties of various glasses can generate $1/f$ noise by modulating either the charge-carrier mobility or concentration. However, both effects have rather insignificant amplitudes that are well below typically measured values.

(2) Electronic DWP can generate $1/f$ noise, most significantly through the mobility modulation leading to realistic Hooge parameters $\alpha\sim 10^{-5}$–10^{-2}; the corresponding concentration modulating mechanism results in much lower α. In both cases α is proportional to the charge-carrier concentration n_c, thus predicting positive non-Ohmic and temperature effects.

(3) The aggregate related Hooge parameter can be in the ballpark of measurable values and is inversely proportional to n_c, thus predicting negative non-Ohmic and temperature effects.

(4) The necessary condition for the generation-recombination mechanism to cause $1/f$ noise is the multiphonon nature of the capture time parameter $\tau_c\propto\exp(E/\varepsilon)$ with ε considerably smaller than both kT and the energy scale of the density of state variations. If these conditions are satisfied, the Hooge parameter due to the generation-recombination mechanism of $1/f$ noise may be in the range of the measured values with $\alpha\propto 1/n_c$ leading to negative non-Ohmic and temperature effects.

TABLE I. Analytical expressions and numerical estimates for the Hooge parameter corresponding to different conceivable mechanisms of $1/f$ noise in chalcogenide glasses. The expressions are given to within the accuracy of numerical multipliers (found in the text of this paper). Experimentally estimated values of the Hooge parameter range (Ref. 30) from 10^{-9} to 10. The meaning of the parameters are as follows: $l\sim 100$ Å is the electron mean-free path, $\Delta\sigma\sim 10^{-17}$ cm^2 is the change in the electron-scattering cross section due to the atomic transition in DWP, $n_c\sim 10^{16}$ cm^{-3} is the charge-carrier concentration, P is the density of states of DWP estimated as $P\sim 10^{18}$–10^{19} for the atomic and 10^{17}–10^{18} eV^{-1} cm^{-3} for the electronic DWP, $D\sim 1$ eV is the interaction potential between the electronic DWP and the trap, $a\sim 10$ Å is the characteristic localization radius of the trap deep in the mobility edge, $N_{\rm eff}\sim 10^{18}$ cm^{-3} is the effective density of states at the mobility edge, $a_0\sim 1$ Å is the characteristic atomic displacement in DWP, $\kappa\sim 10$ is the dielectric permittivity, $\phi\sim 1$–1000 is carrier-concentration enhancement factor due to the electric field, $\varepsilon\sim 0.01$ eV is the scale in the exponential energy dependence of the charge-carrier trapping time, and E_0 is the energy scale of the band tail decay in the mobility gap.

Mechanism	Equation	Estimate
Atomic DWP, mobility	$(l\Delta\sigma)^2 n_c PkT$	10^{-14}–10^{-13}
Atomic DWP, concentration	$\dfrac{D^2Pa^3g(E_F)n_c}{N_{\rm eff}^2}\left(\dfrac{a_0}{a}\right)^6$	10^{-13}–10^{-12}
Electronic DWP, mobility	$\dfrac{(ael)^2 n_c P}{\kappa^2 kT}$	10^{-5}–10^{-2}
Electronic DWP, concentration	$\dfrac{D^2Pa^3g(E_F)n_c}{N_{\rm eff}^2}$	10^{-7}–10^{-6}
Aggregate, concentration	$\dfrac{g(E_F)P(kT)^2}{n_c}\left(\dfrac{e^2}{\kappa E_F}\right)^3$	10^{-5}–10^{-3}
GR concentration	$\dfrac{N_{\rm eff}}{n_c\phi}\dfrac{\varepsilon}{kT}\exp\left(-\dfrac{E_F}{E_0}\right)$	10^{-6}–10^{-2}

Comparing our results with relevant published data on PCM devices, we note that the experimentally estimated Hooge parameter[5] $\alpha\sim 10^{-4}$ is within the domain of our estimates. The observed increase of $\langle(\delta I)^2\rangle/I^2$ with voltage in the non-Ohmic region corresponds to our prediction of the electronic DWP modulated mobility and/or concentration. It was also observed that the relative noise in polycrystalline chalcogenides was orders of magnitude lower than that of their glassy counterparts.[5] We note that, in this connection, DWP in a polycrystal are limited to the grain-boundary regions and their average density is expected to be much lower than in a glass. In addition, the decrease in the degree of disorder that accompanies the phase transition from glass to polycrystalline results in the suppression of $1/f$ noise.

The experimental results presented in Ref. 5 can be explained by the above theoretical results without invoking an avalanchelike multiplication process. An older publication[6] emphasized a rapid increase in $\langle(\delta I)^2\rangle/I^2$ as the voltage approached the threshold value. That observation is qualitatively consistent with the mechanism of electronic DWP modulated mobility and/or concentration assuming that the concentration strongly increases toward switching.

Overall, we conclude that experimentally studying $1/f$ noise can be a valuable source of information about the electronic and atomic properties of chalcogenide phase change memory as viewed against the background of the above developed theory. In particular, the temperature dependence of $1/f$ noise and its high-field non-Ohmic regime can elucidate the underlying mechanisms. Also, we note that, since the localized electronic excitations in this or other form seem to underlie $1/f$ noise in chalcogenide glasses, crossbreed experiments using well absorbed light to vary the electron occupation of localized energy levels may be of significant interest.[40]

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APPENDIX A: DOUBLE WELL POTENTIALS: MOBILITY MODULATION

The spectral properties of the noise for a system of charged particles can be described by the correlation function

$$S_j(\omega) = \langle (\delta j)^2 \rangle_\omega = \langle j \rangle^2 \frac{2\pi\alpha}{N\omega}, \tag{A1}$$

where δj is the fluctuating part of the current density, the subscript ω indicates the Fourier transform, $\langle j \rangle$ is the average current density, N is the number of charge carriers, and ω is the radial frequency.

Our starting point is the Boltzmann equation for nonequilibrium transport

$$\frac{\partial F_\mathbf{p}}{\partial t} + \dot{\mathbf{q}} \cdot \frac{\partial F_\mathbf{p}}{\partial q} + \dot{\mathbf{p}} \cdot \frac{\partial F_\mathbf{p}}{\partial p} = \left.\frac{\partial F_\mathbf{p}}{\partial t}\right|_{\text{coll}}, \tag{A2}$$

where $F_\mathbf{p}$ is the distribution function for the electrons of momentum $\mathbf{p}$, position $\mathbf{q}$, velocity $\dot{\mathbf{q}}$, and force $\dot{\mathbf{p}}$; t is time. The collision term on the right-hand side contains most of the physics specific to a given system. Here we will consider only the current carrying part of the Boltzmann equation and denote the collision term by I. Therefore, Eq. (A2) reduces to

$$e\mathbf{E} \cdot \frac{\partial F_\mathbf{p}}{\partial \mathbf{p}} = I. \tag{A3}$$

The collision term takes the standard form

$$I = \sum_{\mathbf{p}' i} [W^i_{\mathbf{p}p} F_\mathbf{p}(1 - F_{\mathbf{p}'}) - W^i_{\mathbf{p}'p} F_{\mathbf{p}'}(1 - F_\mathbf{p})], \tag{A4}$$

where the sum is over all final momenta and each scattering center i.

We conjecture that some fraction of the scattering centers are DWP which can cause two possible scattering scenarios depending on the atomic configuration at the time of scattering. The transition rate at a DWP site is therefore split into two possibilities given by

$$W^i_{\mathbf{pp}'} = n^i_1 W^{i1}_{\mathbf{pp}'} + (1 - n^i_1) W^{i2}_{\mathbf{pp}'}, \tag{A5}$$

where $W^{i1}_{\mathbf{pp}'}$ is the transition rate due to the atom being in state 1, and the probability that the atom is in state 1 or 2 is given by n_1 and $n_2 = 1 - n_1$, respectively. The occupancy probabilities, n_1 and n_2, of each DWP site varies with time and can be characterized by $n^i_1 = \bar{n}^i_1 + \delta n^i_1$, where $\bar{n}^i_1$ is the mean occupation probability of state 1 and δn^i_1 is the variation of that probability. With this in mind, and by applying Eq. (A5) as well as the fact that for elastic scattering $W^i_{\mathbf{pp}'} = W^i_{\mathbf{p}'\mathbf{p}}$, Eq. (A4) becomes

$$I = \sum_{\mathbf{p}' i} \tilde{W}^i_{\mathbf{pp}'}(F_\mathbf{p} - F_{\mathbf{p}'}) + (W^{i1}_{\mathbf{pp}'} - W^{i2}_{\mathbf{pp}'})(F_\mathbf{p} - F_{\mathbf{p}'})\delta n^i_1, \tag{A6}$$

where $\tilde{W}^i_{\mathbf{pp}'} = \bar{n}^i_1 W^{i1}_{\mathbf{pp}'} + \bar{n}^i_2 W^{i2}_{\mathbf{pp}'} + W^i_{\mathbf{pp}'} \approx W^i_{\mathbf{pp}'}$. The first term in the summation of Eq. (A6) represents the constant part of the collision term I_0 and the second term represents the fluctuating part δI.

In the relaxation-time approximation, the collision term in Eq. (A2) is replaced by $-(F_\mathbf{p} - F_{\mathbf{p}0})/\tau$, where τ is an average relaxation time. This implies that, if left unperturbed, the distribution function will relax to the equilibrium distribution function after a time τ. Inserting the relaxation-time approximation to Eq. (A3) yields

$$F_\mathbf{p} = -\tau e \mathbf{E} \cdot \mathbf{v} \frac{\partial F_\mathbf{p}}{\partial \epsilon}, \tag{A7}$$

where $\mathbf{v}$ is the velocity of the electron and ϵ its energy. Given Eq. (A6) and the fact that,

$$\sum \mathbf{p}' = \frac{V}{(2\pi\hbar)^3} \int d\mathbf{p}', \tag{A8}$$

where $[V/(2\pi\hbar)^3]^{-1}$ is a volume of momentum space (we neglect the factor of 2 associated with two spin states), the constant part of the collision term becomes

$$I_0 = \frac{V}{(2\pi\hbar)^3} \int d\mathbf{p}' W_{\mathbf{pp}'} \tau e (\mathbf{E} \cdot \mathbf{v} - \mathbf{E} \cdot \mathbf{v}') \frac{\partial F_\mathbf{p}}{\partial \epsilon}. \tag{A9}$$

By introducing the angle variables $\angle(\mathbf{v}, \mathbf{E}) = \phi$, $\angle(\mathbf{v}', \mathbf{E}) = \alpha$ and $\angle(\mathbf{v}, \mathbf{v}') = \vartheta$, we see that the transition probability becomes a function of the scattering angle, $W_{\mathbf{pp}'} = W_{\mathbf{pp}'}(\vartheta)$ and that $\cos \alpha = \cos \vartheta \cos \phi + \sin \vartheta \sin \phi \cos \varphi$, where φ is the angle between the planes $(\mathbf{v}, \mathbf{E})$ and $(\mathbf{v}, \mathbf{v}')$. Integrating over the direction of $\mathbf{p}'$ with the angle φ measured from the plane $(\mathbf{v}, \mathbf{E})$, we obtain

$$\int d\mathbf{p}(\mathbf{E} \cdot \mathbf{v}') = \int d\mathbf{p} E v \cos \vartheta \cos \phi = \int d\mathbf{p} \mathbf{E} \cdot \mathbf{v} \cos \vartheta. \tag{A10}$$

Inserting Eqs. (A7) and (A10) into Eq. (A9) yields

$$I_0 = \sum_{p} W_{\mathbf{pp}'}(\vartheta)(1-\cos\vartheta)F_{\mathbf{p}} \equiv \frac{F_{\mathbf{p}}}{\tau}, \tag{A11}$$

where

$$\frac{1}{\tau} \equiv \sum_{\mathbf{p}'} W_{\mathbf{pp}'}(1-\cos\vartheta) \tag{A12}$$

represents the transport relaxation time.

DWP change the distribution function by a small amount $F_{\mathrm{DWP}} \ll F_{\mathbf{p}}$. Using F_{DWP} as a perturbation in the constant part of the collision term and recalling Eq. (A6) gives the following form of the Boltzmann equation:

$$e\mathbf{E}\cdot\frac{\partial F_{\mathbf{p}}}{\partial\mathbf{p}} = -\frac{F_{\mathbf{p}}+F_{\mathrm{DWP}}}{\tau} + \sum_{\mathbf{p}',i}(W^{i1}_{\mathbf{pp}'} - W^{i2}_{\mathbf{pp}'})(F_{\mathbf{p}} - F_{\mathbf{p}'})\delta n^i_1. \tag{A13}$$

For the relaxation-time approximation to hold, the second term and the summation on the right-hand side of Eq. (A13) must cancel each other, which implies that

$$F_{\mathrm{DWP}} = \tau\sum_{\mathbf{p}',i}(W^{i1}_{\mathbf{pp}'} - W^{i2}_{\mathbf{pp}'})(F_{\mathbf{p}} - F_{\mathbf{p}'})\delta n^i_1. \tag{A14}$$

Given the distribution functions one can calculate the constant part j_0 and fluctuating part δj of the current density j using

$$j_0 = \sum_{\mathbf{p}} evF_{\mathbf{p}} \quad \text{and} \quad \delta j = \sum_{\mathbf{p}} evF_{\mathrm{DWP}}, \tag{A15}$$

where v is the electron mean velocity. Inserting Eq. (A14) into δj of Eq. (A15) and replacing $W_{\mathbf{pp}'}$ with the standard transition rate for an energy-conserving transition yields

$$\sum_{\mathbf{p},\mathbf{p}',i} e\tau v\frac{2\pi}{\hbar}[|\langle p|H^{i1}|p'\rangle|^2 - \langle p|H^{i2}|p'\rangle|^2] \times\delta(\epsilon_{\mathbf{p}} - \epsilon_{\mathbf{p}'})(F_{\mathbf{p}} - F_{\mathbf{p}'})\delta n^i_1. \tag{A16}$$

In these matrix elements, the wave functions are normalized to the volume. However, we require a normalization where $W_{\mathbf{pp}'}$ has the dimension of area, which is given by the wave functions[52]

$$\tilde{\psi}_{\mathbf{p}'} = \exp\frac{i}{\hbar}\mathbf{p}'\cdot r \quad \text{and} \quad \tilde{\psi}_{\mathbf{p}} = \frac{1}{\sqrt{v}}\exp\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}, \tag{A17}$$

where v is the velocity. So the former is normalized by the delta function of $\mathbf{p}/(2\pi\hbar)$ while the latter is normalized to the current density for the impeding wave. Therefore, Eq. (A16) becomes

$$\sum_{\mathbf{p},\mathbf{p}',i} e\tau\frac{v^2}{V^2}\frac{2\pi}{\hbar}[|\langle p|H^{i1}|p'\rangle|^2 - \langle p|H^{i2}|p'\rangle|^2] \times\delta(\epsilon_{\mathbf{p}} - \epsilon_{\mathbf{p}'})(1-\cos\varphi)F_{\mathbf{p}}\delta n^i_1, \tag{A18}$$

where the term $(1-\cos\varphi)F_{\mathbf{p}}$ was derived in Eq. (A11). Next, we take into account that $\delta(\epsilon_{\mathbf{p}} - \epsilon_{\mathbf{p}'}) = \delta(p^2 - p'^2)2m$ and replace

$$\sum_{\mathbf{p}'} \to \frac{V}{(2\pi\hbar)^3}2m\int\frac{1}{2}p'd(p'^2)d\Omega'\,\delta(p^2 - p'^2), \tag{A19}$$

where $d\Omega'$ is the elemental solid angle. The integration over p'^2 then amounts to replacing p' by p in the integrand and we obtain

$$\sum_{\mathbf{p},i}\frac{e\tau v^2}{V}\int\frac{mp}{4\pi^2\hbar^4}[|\langle p|H^{i1}|p'\rangle|^2 - \langle p|H^{i2}|p'\rangle|^2] \times(1-\cos\varphi)d\Omega' F_{\mathbf{p}}\delta n^i_1. \tag{A20}$$

We now take into account the expression for the differential cross section,

$$d\sigma = \frac{mp}{4\pi^2\hbar^4}\left|\int\tilde{\psi}^*_{\mathbf{p}'}H\tilde{\psi}_{\mathbf{p}}d\mathbf{r}\right|^2 d\Omega', \tag{A21}$$

in the Born approximation and the definition of the transport cross section[52]

$$\sigma_{\mathrm{tr}} = \int(1-\cos\vartheta)d\sigma. \tag{A22}$$

Combining Eqs. (A21) and (A22) with the expression for the constant part of the current density in Eq. (A15) reduces Eq. (A20) to

$$\delta j = j_0\frac{l}{V}\sum_i(\sigma^{i1}_{\mathrm{tr}} - \sigma^{i2}_{\mathrm{tr}})\delta n^i_1, \tag{A23}$$

where we have used $\tau v = l$, where l is the mean-free path. The only time dependent factor in Eq. (A20) is the variation of the occupancy probability δn^i_1 of the DWP. Consequently, the correlation function of Eq. (A1) is given by

$$S_j(\omega) = \langle(\delta j)^2\rangle_\omega = j^2_0\left(\frac{l}{V}\right)^2\sum_i(\sigma^{i1}_{\mathrm{tr}} - \sigma^{i2}_{\mathrm{tr}})^2\langle(\delta n^i_1)^2\rangle_\omega. \tag{A24}$$

Next we consider the kinetics of the occupation probability of a single well in a DWP. If P_{12} represents the transition rate from well 1 to well 2 and P_{21} represents the opposite transition rate, then in the thermal equilibrium, the time dependence of the variation in the occupation probability can be expressed as

$$\delta n^i_1(t) = \delta n^i_1(0)\exp\left(\frac{-t}{\tau_i}\right), \tag{A25}$$

where τ_i is the characteristic transition time given by $\tau_i = (P^i_{12} + P^i_{21})^{-1}$. According to the binomial distribution, the dispersion of the first factor in Eq. (A25) is given by the product of the means, $\bar{n}^i_1\bar{n}^i_2$. Combining this with the Fourier transform of the second factor yields the correlation function

$$\langle(\delta n^i_1)^2\rangle_\omega = \frac{\bar{n}^i_1(1-\bar{n}^i_1)}{\omega^2 + \tau^{-2}_i}\frac{1}{\tau_i}. \tag{A26}$$

Inserting Eq. (A26) into Eq. (A24) finally results in

$$S_j(\omega)=j_0^2\frac{l^2}{V^{2/3}}\sum_i G_i\frac{\tau_i}{1+(\omega\tau_i)^2}, \tag{A27}$$

where

$$G_i=(\sigma_1^i-\sigma_2^i)^2\bar{n}_1^i(1-\bar{n}_1^i)V^{-4/3} \tag{A28}$$

is the "strength" of the ith fluctuator.

In order to complete the summation over i we specify the results for the DWP model in the high-temperature regime of activation over, rather than tunneling through, the barrier which separates the two wells. If the two local minima of the potential vary by an asymmetry energy E, then the occupation probability for one well is given by

$$\bar{n}_1=\frac{\exp(-E/2kT)}{\exp(-E/2kT)+\exp(E/2kT)}, \tag{A29}$$

where T is the temperature and k is Boltzmann's constant. A DWP is further characterized by the height of the barrier W_B between the wells. The characteristic transition time τ is a function of the barrier height, $\tau=\tau_0\exp(W_B/kT)$. To complete the analysis of Eq. (A27) the discrete sum is converted to an integral by defining a probability density of the DWP as a function of asymmetry energy E and time τ.

The probability distribution has the form given in Eqs. (2) and (7),

$$\rho(E,\tau)=\frac{P}{\tau}. \tag{A30}$$

We also assume that $\sigma_1^i-\sigma_2^i=\Delta\sigma=\text{const}$. With this in mind, inserting Eqs. (A28)–(A30) into Eq. (A27) yields

$$S_j(\omega)=j_0^2\frac{l^2}{V}\frac{P}{4}(\Delta\sigma)^2 \times\int_0^{E_{\max}}\int_{\tau_{\min}}^{\tau_{\max}}dE\,d\tau\frac{1}{(1+\omega^2\tau^2)\left(\cosh\dfrac{E}{2kT}\right)^2}. \tag{A31}$$

Evaluating the integral of Eq. (A31) with the standard DWP model assumptions of $E_{\max}\gg kT$, $\omega\tau_{\min}\ll 1$, and $\omega\tau_{\max}\gg 1$ results in

$$S_j(\omega)=j_0^2\frac{\pi}{4}(l\Delta\sigma)^2\frac{PkTn_c}{N_e}\frac{1}{\omega}, \tag{A32}$$

where the volume has been replaced by $V=n_c/N_e$, with n_c and N_e as the concentration and number of electrons, respectively. Comparing Eq. (A32) to Eq. (A1) provides the following expression for the Hooge parameter,

$$\alpha=\frac{PkTn_c(l\Delta\sigma)^2}{8}. \tag{A33}$$

APPENDIX B: DOUBLE-WELL POTENTIALS: MODULATION OF CARRIER CONCENTRATION

Here we consider in more detail the effect of DWP on modulating electron energy levels in the mobility gap. The modulation of these energy levels causes fluctuations in their occupation number and in the free-carrier concentration. We start with the kinetic equation for a group of energy levels in a narrow energy interval ΔE,

$$\frac{d\Delta N_f}{dt}=-\Delta N_f N_{\text{eff}}\gamma_e+(\Delta N-\Delta N_f)n\gamma_c, \tag{B1}$$

where ΔN_f is the concentration of filled levels and N_{eff} is the effective density of states in the valence (conduction) band. The transition coefficients γ_c and γ_e exhibit temporal fluctuations $\delta\gamma_c$ and $\delta\gamma_e$ caused by the energy-level modulation $E\to E+\delta E$. We express the latter modulation as

$$\delta E=\sum_i D_i\delta n_1^{(i)}, \tag{B2}$$

where D_i and $\delta n_1^{(i)}$ are the coupling parameter and the occupation numbers of ith DWP, and summation over all DWP is implied.

Taking into account that

$$\gamma_c=\gamma_0\exp(-E/\varepsilon),\quad \gamma_e=\gamma_0\exp[-E(1/\varepsilon+1/kT)],$$

the corresponding fluctuations become

$$\delta\gamma_c=(\gamma_c/\varepsilon)\sum_i D_i\delta n_1^{(i)},\quad \delta\gamma_e=\gamma_e(1/\varepsilon+1/kT)\sum_i D_i\delta n_1^{(i)}. \tag{B3}$$

Linearizing Eq. (B1) with respect to fluctuations $\delta\gamma_c$, $\delta\gamma_e$, and δN_f yields

$$\frac{d\delta N_f}{dt}+\frac{\delta N_f}{\tau}=-\Delta N_f N_{\text{eff}}\delta\gamma_e+(\Delta N-\Delta N_f)n\delta\gamma_c. \tag{B4}$$

Implementing the equilibrium relation $\Delta N_f N_{\text{eff}}\gamma_e=(\Delta N-\Delta N_f)n\gamma_c$ and substituting expressions for $\delta\gamma$ from Eq. (B3) gives the final kinetic equation

$$\frac{d\delta N_f}{dt}+\frac{\delta N_f}{\tau}=n(\Delta N-\Delta N_f)\gamma_c\sum_i\frac{D_i}{kT}\delta n_1^{(i)}. \tag{B5}$$

Here the sum on the right-hand side represents a random quantity. If Eq. (B5) is written in the terms of a change per center, $(\delta N_f/\Delta N)$, then the latter sum represents the effect of a random DWP environment on a given center.

Performing the Fourier transform yields

$$(\delta N_f)_\omega=\frac{\tau n(\Delta N-\Delta N_f)\gamma_c}{1+i\omega\tau}\sum_i\frac{D_i}{kT}\delta(n_1^{(i)})_\omega. \tag{B6}$$

Taking into account the relationships

$$\tau_c=\frac{1}{\gamma_c n},\quad \frac{\Delta N-\Delta N_f}{\tau_c}=\frac{\Delta N_f}{\tau_e}=\frac{\Delta N}{\tau_e+\tau_c}=\frac{\Delta N}{\tau_c}(1-f),$$

and using

$$f(1-f)=kT\frac{\partial f}{\partial E},$$

Equation (B6) can be written in the form

$$\frac{(\delta N_f)_\omega}{\Delta N} \equiv \delta f = \frac{\partial f}{\partial E}(\delta E)_\omega, \tag{B7}$$

where δf is the change in the occupation number that is a maximum,

$$(\delta f)_{\max} = \frac{(\delta E)_\omega}{4kT},$$

at $E=E_F$, and where we have introduced the Fourier transform of the effective energy fluctuation

$$(\delta E)_\omega = \frac{1}{1+i\omega\tau}\sum_i D_i \delta(n_1^{(i)})_\omega. \tag{B8}$$

Because the product $f(1-f)$ is a sharp maximum of width kT at the Fermi energy, the number of significantly contributing electron centers can be estimated as

$$\Delta N_T \approx g(E_F)kT.$$

We then neglect the term $\omega\tau$ in the denominator reflecting the fact that the electron states are relatively shallow and have rather short relaxation times; hence

$$(\delta f)_{\max} = \sum_i \frac{D_i}{4kT}\delta(n_1^{(i)})_\omega \tag{B9}$$

The latter random quantity characterizes an arbitrary electron center with a given two-level system (TLS) pattern in its proximity.

The dispersion in the number of charged carriers localized on $\Delta N_T V$ electron centers is estimated as

$$\begin{aligned}\Delta N_T V\langle[(\delta f)_{\max}]^2\rangle &= \Delta N_T V \sum_i \left\langle \left(\frac{D_i}{4kT}\right)^2 [\delta(n_1^{(i)})]^2_\omega \right\rangle \\ &\approx \Delta N_T V N_{\mathrm{TLS}} R^3 \left\langle \left(\frac{D}{4kT}\right)^2 \right\rangle \langle[\delta(n_1^{(i)})]^2_\omega\rangle,\end{aligned} \tag{B10}$$

where we have introduced the average number of two-level systems $N_{\mathrm{TLS}}R^3$ in the volume of the localized electron wave function, and approximately decoupled the frequency dependent fluctuations in TLS occupation numbers from the static interaction parameters D_i.

The latter quantity is directly related to the dispersion in the number of charge carriers. Indeed, the above used condition $\omega\tau \ll 1$ means that important localized charge carriers are in the state of thermal equilibrium. Correspondingly, the change in the occupation number of the free carriers is by the factor $\exp(-E_F/kT)$ smaller than $\Delta N_T V\langle[(\delta f)_{\max}]^2\rangle$. Its relative value, of primary interest here, is given by

$$\frac{\langle(\delta I)^2_\omega\rangle}{I^2} = \frac{\langle(\delta n)^2_\omega\rangle}{n^2} = \frac{\Delta N_T N_{\mathrm{TLS}} R^3}{N_{\mathrm{eff}}^2 V}\left\langle \left(\frac{D}{4kT}\right)^2 \right\rangle \langle[\delta(n_1^{(i)})]^2_\omega\rangle, \tag{B11}$$

where we have expressed the average number of free carriers as $N_{\mathrm{eff}}V\exp(-E_F/kT)$.

We use the already described procedure of averaging [see Eqs. (A31) and (A32)]

$$N_{\mathrm{DWP}}\langle[\delta(n_1^{(i)})]^2_\omega\rangle = \frac{\pi}{4}\frac{PkT}{\omega}.$$

As a result we get the $1/f$ noise spectrum in the form of

$$\frac{\langle(\delta I)^2_\omega\rangle}{I^2} = \frac{\pi}{4}D^2 P a^3 g(E_F)\frac{\Delta\omega}{\omega V N_{\mathrm{eff}}^2}. \tag{B12}$$

Its corresponding Hooge parameter is given by

$$\alpha = \frac{D^2 P a^3 g(E_F) n_c}{8N_{\mathrm{eff}}^2}. \tag{B13}$$

APPENDIX C: GENERATION-RECOMBINATION NOISE

Following Ref. 53, a partial electric current fluctuation related to a group of trap levels of certain energy, is given by

$$\delta I = \frac{I}{n_c V}\nu, \tag{C1}$$

where ν is the average number of electron emissions from that level per unit time; the multiplier $I/(n_c V)$ gives the current per carrier whose average concentration in volume V is n_c.

Consider electron (hole) levels in a small energy interval ΔE. They can be treated as a monoenergetic level of concentration $\Delta N(E)=g(E)\Delta E$. Let ΔN_f be the equilibrium concentration of filled energy levels in that same interval. It is determined by the balance equation

$$\frac{\Delta N_f}{\tau_e} = \frac{\Delta N - \Delta N_f}{\tau_c}, \tag{C2}$$

where τ_e is the time constant for emission from a filled level, and τ_c is the time constant for the capture by an empty level.

A useful relationship between τ_e and τ_c follows when the corresponding rates are written as $\Delta N_f N_{\mathrm{eff}}\gamma_e$ and $(\Delta N - \Delta N_f)n_c\gamma_c$, respectively, where N_{eff} is the effective density of states in the valence (conduction) band. The coefficients γ_e and γ_c do not depend on the particle concentrations, and their ratio $\gamma_e/\gamma_c=\exp(-E/kT)$ is found from the equilibrium relations $n_c/N_{\mathrm{eff}}=\exp(-E_F/kT)$ and $\Delta N_f/(\Delta N-\Delta N_f)=\exp[(E-E_F)/kT]$. As a result

$$\tau_e/\tau_c = \exp[-(E_F-E)/kT],$$

which translates into

$$\tau = f\tau_c \quad \text{with} \quad f=\{1+\exp[(E_F-E)\ /kT\}^{-1}. \tag{C3}$$

If the concentration of filled levels is slightly perturbed from equilibrium by δN_f, it relaxes back to ΔN_f according to

$$\frac{d\delta N_f}{dt} = -\frac{\delta N_f}{\tau} \quad \text{with} \quad \frac{1}{\tau} = \frac{1}{\tau_e} + \frac{1}{\tau_c}, \tag{C4}$$

where t is time. The corresponding temporal dependence $\delta N_f \propto \exp(-t/\tau)$ translates into the current fluctuations caused by one trapping/detrapping event decaying similarly as

$$\delta I(t) = (I/n_c V)\nu \exp(-t/\tau).$$

Its frequency component is

$$\delta I(\omega) = 2\int_0^\infty \delta I(t)\exp(i\omega t)dt = \frac{2I\tau}{n_c V(1+i\omega\tau)}. \quad \text{(C5)}$$

Since the average number of emissions per second is

$$\nu = \frac{\Delta N_f V}{\tau_e} = \frac{\Delta N V}{\tau_e + \tau_c}, \quad \text{(C6)}$$

the relative partial noise spectrum becomes

$$\frac{\langle(\delta I)^2\rangle}{I^2} = \nu\frac{(\delta I)^2}{I^2} = \frac{4\Delta N\tau^2}{n_c^2 V(\tau_e+\tau_c)(1+\omega^2\tau^2)}, \quad \text{(C7)}$$

where the angle brackets indicate the Fourier transform. Integrating the latter result over the band tail spectrum yields Eq. (26).

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*vkarpov@physics.utoledo.edu

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