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Lucky-drift model for avalanche multiplication in amorphous semiconductors

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A new model for avalanche carrier multiplication in amorphous semiconductors is suggested. In contrary to previous considerations, the model does not employ the Shockley's lucky-electron ansatz according to which a free carrier gains the energy from electric field in a ballistic motion. We show that the majority of free carriers reaching the ionization threshold energy do so by drift, not ballistically.

1 Introduction

The process of avalanche multiplication of charge carriers in amorphous semiconductors, particularly in amorphous selenium (a-Se), known since many years [1, 2, 3, 4] has received recently a significant attention of the scientific community due to the application of these materials in X-ray imaging devices [5, 6, 7]. It has been well established experimentally [4, 5] that the avalanche phenomenon is observed in a-Se at electric fields above $\sim 8 \times 10^5$ V/cm. However, there is still no generally accepted explanation of this effect.

The most important quantitative characteristic for charge multiplication phenomena is an impact ionization rate defined as the number of carriers generated per unit distance by impact ionization by one injected (photogenerated) carrier as it moves through the medium. It is widely believed that holes and not electrons are responsible for the impact ionization in a-Se since they possess a higher mobility than electrons. The impact ionization rate strongly depends on the applied electric field. It has already become a tradition to fit experimental results for impact ionization rate as a function of applied electric field, F, in the form

$$\beta = \beta_0 \exp\left(-\frac{F_0}{F}\right), \tag{1}$$

where β_0 and F_0 are parameters, which should be fitted to experimental data.

Shockley first treated the parameters in Eq. (1) [8]. He just supposed that if an electron attains some sufficient energy E_i it is able to generate an electron-hole pair via the impact ionization process. Shockley's theory gives no explanation for the ionization threshold energy, E_i. It is kept as a parameter to be fitted to experimental data. Shockley assumed that free carriers gain energy in their ballistic motion in the extended band states. In such a motion the carrier is supposed to avoid any scattering processes until it attains the ionization threshold energy E_i from electric field. In other words a charge carrier has to traverse the

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distance E_i/eF without any scattering events. The probability density for a charge carrier to attain energy E via such a process is determined by the Poisson distribution

$$f(E) = \frac{1}{eF\lambda} \exp\left(-\frac{E}{eF\lambda}\right). \tag{2}$$

Here λ is the mean free path, and $eF\lambda$ is the energy gained by a carrier moving ballistically over the distance λ in the electric field F. Resulting ionization rate is the product of the average number of scattering events per unit distance and the probability to attain the threshold energy E_i

$$\beta = \lambda^{-1} \exp\left(-\frac{E_i}{eF\lambda}\right). \tag{3}$$

Equation (3) has the same form as Eq. (1). Fitting Eq. (3) to experimental data for impact ionization rate for holes in a-Se obtained in Ref. [5], one gets the following values of the involved parameters: $\lambda = 0.6$ nm and $E_i = 0.55$ eV [9]. Surprisingly, the value of the energy threshold, E_i, for impact ionization appears to be approximately four times less than the band gap $E_g \approx 2$ eV in a-Se. Such a low energy threshold indicates that the ionization process involves some localized states in the mobility gap of the amorphous semiconductor.

Arkhipov and Kasap [9] improved the Shockley's model by taking the gap states into account. They assumed that the secondary electron and hole produced in the impact event are generated in the localized gap states. Arkhipov and Kasap considered the thermally assisted dissociation of already generated electron-hole pairs from the localized states. They also assumed, following Shockley [8], that free carriers gain energy in their ballistic motion in the extended band states. However, it has been already shown for crystalline semiconductors that the vast majority of free carriers reach the ionization threshold energy not in the ballistic motion, but rather by drift [10, 11] in a process that has to be known the "lucky drift" model.

In amorphous semiconductors, the probability of scattering events is much higher than in crystalline materials and hence the lucky-electron ballistic motion suggested by Shockley is less probable than in the crystalline counterparts. Therefore we find it reasonable to analyze the possibility of gaining energy for a free carrier in amorphous semiconductor not only ballistically, but also via its motion with scattering on disorder potential and on phonons. We will show below that the latter process in amorphous semiconductors is more probable than a ballistic gain for the necessary ionization threshold energy. Furthermore, we extend the model of Arkhipov and Kasap by considering the generation of secondary carriers not only in the localized states, but also with creation of one of these secondary carriers in the extended states.

The main result of our paper is the field dependence of the impact ionization rate based on including numerous scattering events of a moving charge carrier on disorder potential and phonons. In Section 2 we consider the two possibilities to excite the secondary charge carrier into the localized state with higher energy or into the band state in the framework of a ballistic motion of the primary carrier. It will be shown that in the framework of the ballistic primary carrier motion both models are not able to provide a quantitative agreement with experimental data. In Section 3 we develop a new "lucky-drift" model for the avalanche multiplication in amorphous semiconductors by taking into account the drift and not the ballistic energy gain of primary charge carriers along with the possibility to excite the secondary charge carrier in the impact collision event from a localized state directly into the band state. We also compare theoretical results with experimental data and show that our model is well able to fit experimental data quantitatively.

2 Ballistic models

2.1 Sub-gap ionization

The typical band gap structure of an amorphous semiconductor is shown in Fig. 1a. The density of states (DOS) includes tail states near the valence and the conduction band edges as well as the peak related to

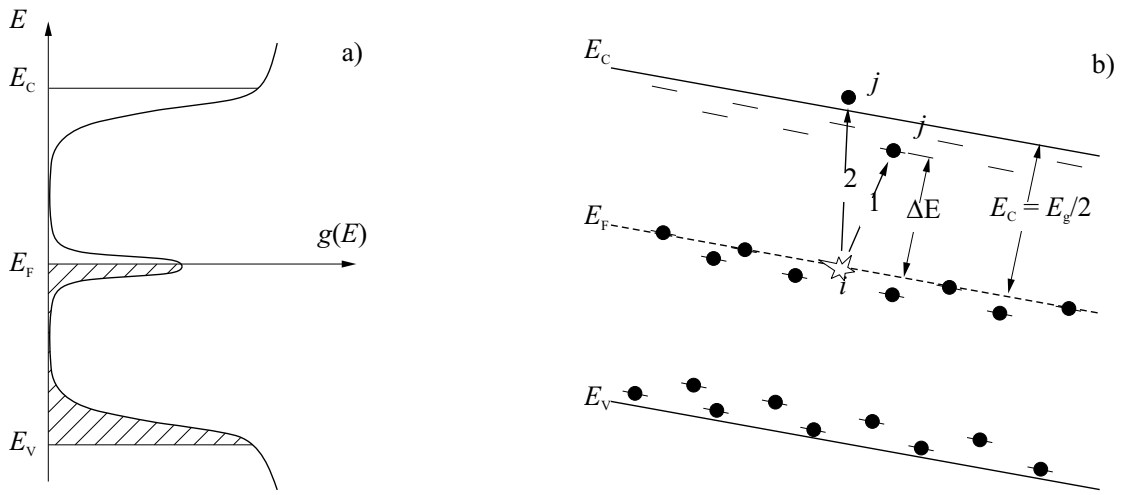

Fig. 1 Schematic diagrams for the density-of-states in amorphous semiconductor (a) and for two possible ionization processes (b): 1 - sub-gap ionization; 2 - gap-to-band ionization.

various disorder-induced defects at the middle of the mobility gap [12]. The Fermi level, E_F, is located in the middle of the band gap. In further calculations, the origin of the energy axis will be put at the Fermi level with the positive direction toward the mobility edge of the conduction band, E_c.

The process of sub-gap ionization corresponds to the tunnelling of a carrier from a localized site i near the Fermi level E_F to an empty localized site j in the band tail (see Fig. 1b, process 1). For simplicity we will consider electrons as the avalanche charge carriers keeping in mind that the theory can be also applied for avalanche creation of holes by replacing the corresponding notations. Such a sub-gap transition is only possible if an exciting free primary carrier attains a sufficient energy $\Delta E = E_j - E_i$. The probability density $f(E)$ to attain the energy E is described by Eq. (2). Since the transition of the secondary electron occurs between two localized states separated in space by some distance r_{ij}, its probability $W(E)$ is determined by the overlap integral between the wave functions of the localized states. The secondary electron-hole pair created in the localized states can either recombine geminately, or it can dissociate. It is the dissociation probability, $\eta(E)$, of such a pair that was the subject of the study of Arkhipov and Kasap [9]. The sub-gap impact ionization rate for the creation of both localized carriers (electron and hole) in the localized sub-gap states has the form

$$\beta_{SG} = \int_0^{E_c} dE \, \frac{1}{l(E)} f(E) W(E) \eta(E). \tag{4}$$

Here $l(E) = E/eF$ is the path length that a carrier should traverse in the direction of the electric field in order to attain the energy E.

The transition probability (overlap integral) between two sites separated by distance r_{ij} for states with localization radius α is proportional to $\exp(-2r_{ij}/\alpha)$. The probability density to find the nearest neighbour site at a distance r has the Poisson form $4\pi N r^2 \exp\left(-\frac{4\pi}{3} N r^3\right)$ for a random distribution of sites with concentration N in three-dimensional space. The product of the overlap integral and this probability density has a sharp maximum at $r = \alpha$. Hence the decisive contribution to the impact generation process comes from sites separated by a distance of the order of the localization length α. Therefore the transition probability can be written as

$$W(E) \approx \mathrm{e}^{-2} \int_0^{\alpha} dr \; 4\pi N(E) r^2 \exp\left[-\frac{4\pi}{3} N(E) r^3\right] = \mathrm{e}^{-2} \left\{1 - \exp\left[-\frac{4\pi}{3} N(E) \alpha^3\right]\right\}. \tag{5}$$

Table 1 Results for the impact ionization rate (cm^{-1}) calculated from different models

Electric field, MV/cm	Sub-gap ionization via ballistic motion from Eq. (4)[1]	Gap-to-band ionization via ballistic motion from Eq. (9)[2]	Gap-to-band ionization via lucky-drift from Eq. (16)[3]	Experimental data for holes in a-Se from [4]
0.5	6.4×10^{-7}	2.2×10^{-6}	0.006	—
0.8	0.004	0.05	320	200
1.0	0.1	1.9	8.2×10^{3}	2×10^{3}
1.2	0.7	20.7	5.9×10^{4}	8×10^{3}
1.6	10	433	5.2×10^{5}	4×10^{4}

[1] $E_c = 0.8$ eV, $\lambda = 0.6$ nm, $N_0\alpha^3 = 0.1$, $E_0 = 0.025$ eV, and $\eta(E) = 1$.
[2] $E_c = 0.8$ eV and $\lambda = 0.6$ nm.
[3] $E_c = 0.8$ eV, $\lambda_{el} = 0.6$ nm, $\lambda_{ie} = 6\lambda_{el}$, and $E_r = 0.04$ eV.

Here $N(E)$ is the concentration of localized states with energies below E

$$N(E) = \int_{-\infty}^{E} dE'\; g(E') = N_0 \exp\left(\frac{E - E_c}{E_0}\right), \tag{6}$$

assuming the exponential DOS in the tail of the conduction band

$$g(E) = \frac{N_0}{E_0} \exp\left(\frac{E - E_c}{E_0}\right). \tag{7}$$

In Eq. (7) N_0 denotes the total concentration of localized states, and E_0 is the energy scale. Since $N_0\alpha^3 \ll 1$ one can rewrite Eq. (5) in the more convenient form

$$W(E) \approx \mathrm{e}^{-2} \frac{4\pi}{3} N_0 \alpha^3 \exp\left(\frac{E - E_c}{E_0}\right). \tag{8}$$

Results for the impact ionization rate calculated from Eq. (4) for reasonable material parameters are given in Table 1. For simplicity we assume in the calculations $\eta(E) = 1$. Even for such a favorable efficiency for the pair dissociation, it is evident that no avalanche multiplication can be observed under experimental conditions. For example, at the enormously high electric field with the strength 1.6 MV/cm one has $\beta_{SG} = 10\ \mathrm{cm}^{-1}$. Such a low ionization rate is not enough to generate a single secondary carrier by a primary one passing trough a sample of 50 μm thickness. The reason for such a low ionization efficiency is the extremely low transition probability $W(E)$ for creation of a secondary electron-hole pair in the tunnelling process between two localized states.

2.2 Gap-to-band ionization

An alternative process to the creation of the secondary electron-hole pair in the localized states is the direct excitation of a secondary electron into extended states above the mobility edge. Such a process is shown in Fig. 1b by arrow 2. In this process the transition probability does not suffer from a smallness of the overlap integral which was the case in the tunnelling process. Considering the direct excitation of the secondary electron into extended states one should not care about the dissociation probability, $\eta(E)$, since a free secondary carrier created in a strong electric field quickly escapes from the creation place and herewith it avoids the geminate recombination. One can express the ionization rate for the direct impact activation of a secondary electron into the conduction band in the form

$$\beta_{GB} = \int_{E_c}^{\infty} dE\; \frac{1}{l(E)} f(E). \tag{9}$$

Results for the impact ionization rate evaluated from Eq. (9) are shown in Table 1. The impact ionization rates for gap-to-band excitation are higher than for the sub-gap one by at least an order of magnitude. However, β_{GB} is still too small to provide the avalanche effect even at such a high field as $F = 1.2$ MV/cm. Therefore aiming at the explanation of experimental data one has to examine the Shockley's assumption for the energy gain by the primary electrons. In fact, it is already well known for crystalline semiconductors that the ballistic mechanism employed above strongly underestimates the number of the primary electrons reaching the ionization threshold energy necessary for the avalanche multiplication [10, 11]. It was one of the reasons that led researchers to developing the lucky drift model for impact ionization in crystalline semiconductors. Below we suggest for the first time a new lucky-drift model for amorphous semiconductors.

3 Lucky-drift model for amorphous semiconductors

3.1 Scattering formalism

In the Shockley's model [8] used so far for description of the avalanche multiplication in amorphous semiconductors it is presumed that a free carrier accelerated by electric field gains its energy in a purely ballistic collisionless motion. However, the later studies have shown that a more probable mechanism to gain the energy necessary for the impact ionization is related to drift of primary charge carriers [10, 11]. The corresponding model of the energy gain is known as a lucky-drift model. So far this model has been developed only for crystalline semiconductors without taking into account the scattering of primary charge carriers on the disorder potential. Only collisions with phonons were considered. In what follows we will extend this lucky-drift model to the amorphous semiconductors by taking into account the collisions of charge carriers on both phonons and disorder potential. Therefore two kinds of scattering mechanisms will be considered here: elastic scattering on disorder potential and inelastic collisions with phonons. Possible elastic collisions with phonons will be neglected.

In Fig. 2 a schematic trajectory of a primary charge carrier is shown. Elastic and inelastic collisions are indicated by filled and open circles respectively. The elastic scattering process is characterized by the mean free path λ_{el}. In amorphous materials λ_{el} is of the order of an interatomic spacing, i.e. it should be about 0.3 to 0.6 nm. In the elastic process, the scatters are distributed randomly in space and the scattering angle after each collision event can be also treated as random. Inelastic scattering is described by the mean free path λ_{ie}. For simplicity we will assume that the energy loss of a primary charge carrier in each collision with phonons is characterized by the constant amount E_r. We assume that this energy is equal to the optical phonon energy, e.g. $E_r \approx 0.04$ eV in a-Se. We also assume that collisions with phonons do not change the carrier trajectory essentially. In the following section a theory of the energy gain is developed in the framework of this model.

3.2 Energy gain

When treating elastic scattering events in the following we will always distinguish between "lucky" collisions and "unlucky" ones. After a lucky elastic collision, the velocity of a primary carrier has a positive projection on the field direction and hence the carrier gains energy from the electric field after the scattering event. The scattering angle θ defined here as the angle between the carrier velocity after the collision event and the field direction should fulfill the inequality $\theta < \pi/2$ for lucky collisions. In the opposite case, $\theta > \pi/2$, a carrier loses its energy travelling against the field. The transition between these two regimes (loss and gain) corresponds to the angle $\theta_c = \pi/2$.

Consider an arbitrary path of a primary charge carrier as a series of k elastic collisions and m inelastic ones. Assume the number of lucky collisions in such a path is k_l, and the number of unlucky collisions is k_u. The energy gain (or loss) in this series of collisions can be approximated in the form

$$E_a \approx k_l eF\lambda_{el}\langle\cos\theta\rangle + k_u eF\lambda_{el}\langle\cos\theta^*\rangle - mE_r. \tag{10}$$

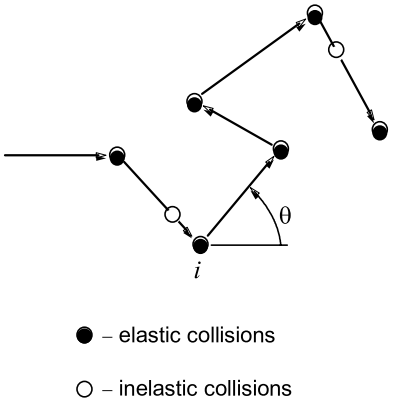

Fig. 2 Possible scattering trajectory of a primary carrier.

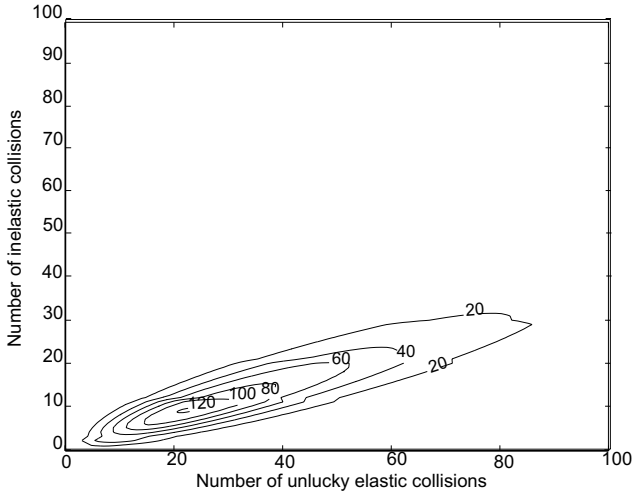

Fig. 3 Impact ionization rate (cm^{-1}) as a function of collision numbers. Calculation parameters: $F = 1.2$ MV/cm, $E_c = 0.8$ eV, $\lambda_{el} = 0.6$ nm, $\lambda_{ie} = 6\lambda_{el}$, and $E_r = 0.04$ eV.

Here $\langle\cos\theta\rangle$ and $\langle\cos\theta^*\rangle$ are the projections of the unit velocity vector on the electric field direction averaged over lucky and unlucky scattering events, respectively (see Appendix A for details).

If the energy E_a is given, one can evaluate from Eq. (10) the number of lucky collisions, k_l, provided m and k_u are also given. In the following we will assume E_a to be equal to the ionization threshold energy E_c necessary to excite a secondary charge carrier from the Fermi level in the mobility gap to the band edge. The probability to acquire the energy E_c in the described way is the product of a probability $P_{el}(k_u)$ to have k_u unlucky events in the chain of k elastic scattering events and a probability $P_{ie}(k,m)$ to have m inelastic collisions in the same chain. Assuming the set of collision events to be Markovian, one can approximate these probabilities by Poisson formulas

$$P_{el}(k_u) = \frac{[k(1-W_1)]^{k_u}}{k_u!}\exp[-k(1-W_1)], \tag{11}$$

and

$$P_{ie}(k,m) = \frac{(k\lambda_{el}/\lambda_{ie})^m}{m!}\exp(-k\lambda_{el}/\lambda_{ie}). \tag{12}$$

Here $W_1 = 1/2$ is the probability for a carrier to be reflected with the angel $\theta \le \pi/2$ (see Appendix A for details). The resulting probability to acquire the energy E_c via a certain combination of collisions is

$$P(k_u,m) = P_{el}(k_u)P_{ie}(k,m). \tag{13}$$

In the next section, Eqs. (10)–(13) will be used to calculate the impact ionization rate.

3.3 Ionization rate

In order to determine the ionization rate from Eqs. (10)–(13), one has to evaluate the length of the primary carrier path in the field direction that corresponds to each particular number of the elastic scattering events. After performing $k = k_l + k_u$ elastic collisions a carrier traverses in the field direction a distance l of the order

$$l(k) \approx \lambda_{el}(k_l\langle\cos\theta\rangle + k_u\langle\cos\theta^*\rangle). \tag{14}$$

Then the impact ionization rate for a given combination of collision numbers k_u and m is

$$\beta(k_u, m) = \frac{P(k_u, m)}{l(k)}. \tag{15}$$

Using Eqs. (10)–(15) we calculate now the impact ionization rate as a function of the collision numbers k_u and m. Figure 3 shows as an example the corresponding results for $F = 1.2$ MV/cm. The rate demonstrates a pronounced maximum in a particular region of k_u and m. The position of the maximum and its height depend on the applied electric field. With increasing F, the maximum becomes more pronounced and it shifts toward the lower collision numbers.

The resulting impact ionization rate for lucky-drift model should include all possible combinations k_u and m in the form

$$\beta_{LD} = \sum_{m=0}^{\infty} \sum_{k_u=0}^{\infty} \beta(k_u, m). \tag{16}$$

Results for the impact ionization rate, β_{LD}, calculated from Eq. (16) are given in Table 1. It is evident that β_{LD} demonstrates the abrupt transition to the avalanche regime at $F \approx 0.8$ MV/cm. This is the main result of our theory. The value of the impact ionization rates for two ballistic models described above are also shown in the table. It is well seen that the lucky-drift model developed in this work provides a better fit to experimental data than other theories.

In this paper we have not yet addressed the temperature effect on the avalanche multiplication in amorphous semiconductors recently considered by Arkhipov and Kasap [9]. Experimental data indicate a slight increase of the ionization rate with temperature [4]. This effect in a-Se is not very pronounced. The ionization rate for holes changes only by a factor of two when temperature changes from 300 K to 150 K. We believe that such a week dependence could be explained by taking into account the real Fermi distribution of localized charge carriers in the mobility gap. In the above consideration we assumed that the ionization threshold energy E_c necessary to excite the secondary charge carrier is temperature-independent being equal to the energy distance between the mobility edge and the Fermi level. With rising temperature, the states above and below the Fermi level become more populated by electrons and holes respectively, which should diminish the excitation energy for the secondary carriers and hence it should lead to the increase of the ionization rate with temperature.

4 Conclusions

A new lucky-drift model is suggested for the avalanche carrier multiplication in amorphous semiconductors. The main difference of the present model with respect to the previous theories for amorphous semiconductors is the exclusion of Shockley's assumption on the ballistic motion of the primary injected or photoexcited carriers. In the present model, scattering of such carriers are taken into account and it is shown that lucky-drift energy gain is more favourable than the ballistic motion. Lucky drift is able to build up sufficient energy to ionize a carrier from localized states near the Fermi level to the transport band. The results of the present model are in good agreement with experimental data on avalanche multiplication in a-Se.

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A Appendix

The surface element dS of a sphere of radius r in spherical coordinates θ and ϕ has the form

$$dS = rd\theta \times r\sin\theta d\phi. \tag{17}$$

The directions for elastic scattering of carriers are assumed random. Hence the probability for a primary carrier to be reflected under the angle $\theta < \theta_c$ can be expressed as a ratio of a spherical surface area $S(\theta_c)$ determined by the polar angle θ changing between 0 and θ_c to the total surface area. The surface area $S(\theta_c)$ is

$$S(\theta_c) = \int_0^{\theta_c}\int_0^{2\pi} d\theta d\phi\, r^2\sin\theta = 2\pi r^2(1-\cos\theta_c). \tag{18}$$

Hence the probability for a carrier to be reflected under the angle $\theta < \theta_c$ is

$$W_1(\theta < \theta_c) = \frac{2\pi r^2(1-\cos\theta_c)}{4\pi r^2} = \frac{1}{2}(1-\cos\theta_c). \tag{19}$$

In order to average $\cos\theta$ one needs a probability density $f(\theta)$ for a primary carrier to be reflected in lucky collision with a certain angle θ. Since all directions are equally probable, the corresponding probability density can be expressed in the form

$$f(\theta)\, d\theta = \frac{2\pi r\sin\theta \times r\, d\theta}{S(\theta_c)}. \tag{20}$$

Averaging $\cos\theta$ over the polar angle θ in the range between 0 and θ_c one can express the result in the form

$$\langle\cos\theta\rangle = \int_0^{\theta_c} d\theta\ \cos\theta f(\theta) = \frac{1}{2\pi(1-\cos\theta_c)}\int_0^{\theta_c} d\theta\, 2\pi\cos\theta\sin\theta \equiv \frac{1+\cos\theta_c}{2}. \tag{21}$$

For unlucky collisions ($\theta_c < \theta < \pi$) one obtains in the similar way the expression

$$\langle\cos\theta^*\rangle = \frac{\cos\theta_c - 1}{2}. \tag{22}$$

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