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A Quantum-physical Approach to Modelling the Failure Rate of a Two-state Component

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The objective of the thought experiment in this contribution is to explore the potential of the well-known theory of quantum physics in terms modelling the physics of failure as part of reliability engineering. The approach is based on Fermi's golden rule predicting the transition rate from an initial state to a final state under the influence of a weak perturbation relative to a given time interval. The transition rate fits brilliantly into the framework of reliability engineering and reliability modelling as the *MTTF* can be derived easily. As we are scaling down from classical (macro) hardware to photons, the *MTTF* is scaling down from hours to attoseconds. The interpretation of results shows that the relations between the incoming perturbation energy and the resulting transition rate are pretty familiar compared to macro effects.

Keywords: quantum physics, physics of failure, reliability modelling, semiconductor.

1. Introduction

The upcoming lithography process in the semiconductor industry is gradually moving down to 2 nanometers. Increasingly complex circuits can be implemented on silicon with increasingly density. This shifts semiconductor technology from the framework of electronics to the laws of quantum physics.

Here is an example: Silicon carbide crystals form more than 250 polytypes, see Cheung (2006). For the sake of simplicity, let us discuss the 3C-SiC type, which is cubic with all faces centred as a diamond structure (Pearson symbol cF8). The lattice constants are equal with

$$a = c = 435.96 \text{ pm} , \quad (1)$$

refer to Park et al. (1998). In relation to the semiconductor industry's ability to produce 2 nm structures, this means that the crystals have a width of about five molecules.

Consequently, the level of detail in reliability modelling must be adjusted accordingly in order to obtain dependable quantified statements. The level of detail is shifted from roughly modelled components (refer to Section 4.1) up to – or down to, depending on the point of view – molecules, atoms, and electrons.

The objective of the thought experiment in this contribution is to explore the potential of the well-known theory of quantum physics in terms modelling the physics of failure as part of reliability engineering. We discuss a single molecule of a silicon carbide semiconductor. In terms of reliability modelling a two-state model is considered, assigning the property either functioning or faulty to the item discussed.

2. The State of Research

The denotation *quantum reliability* is interpreted in three different ways:

(1) The reliability assessment of *quantum devices* as part of the emerging quantum technology, refer to Cui (2023).

Typical examples are quantum circuits (especially qubits), quantum gates, and quantum information transmission, refer to Giusto et al. (2023), Safaei et al. (2024), and Lin et al. (2019).

(2) The application of *quantum computing* in reliability assessment.

This is where quantum algorithms are applied to optimization tasks, system simulations, and data processing. It is understood as a combination of classical and quantum computing strengths, quantum-enhanced machine learning and simulation, refer to Yazdi (2024).

(3) Reliability assessment discussing *quantum physical* effects.

Lin et al. (2020) present a non-Hermitian quantum approach to the reliability of a two-state system. They are "giving a Hilbert structure to the system states, then utilize a non-Hermitian Schrödinger equation to describe the state evolution and finally derive two new lifetime distributions."

We would like to add a simple approach to the third category by applying Fermi's Golden rule just to model the *physics of failure* on the level of photons, electrons, atoms, molecules, and crystals. We see semiconductors as the main application area in terms of functional safety and reliability engineering.

3 Some notes on quantum physics

Quantum physics – based on the fundamental theory of quantum mechanics, refer to Feynman et al. (1964) – models among others the properties of photons, electrons, atoms, and molecules. As indicated in the introduction, these items are becoming increasingly interesting for reliability modelling.

Observations at this level are expressed by wave functions, which provide information in the form of probability amplitudes – a very familiar environment in terms of safety and reliability engineering. The wave function of a particle is calculated by solving the Schrödinger equation, where the eigenvalues, the eigenstates, and finally the eigenfunction are calculated, refer to Holzner (2020). Many quantum aspects cannot be solved exactly; therefore, they are modelled applying approximation methods. We apply three approximation methods here:

- The Fermi gas (see Section 3.1)
- Fermi's golden rule (see Section 3.2)
- The perturbation theory, refer to Holmes (2013)

We are discussing a minor perturbation caused by a photon and leave the perturbation term suffi–ciently small according to Holzner (2015).

3.1 *The Fermi Gas*

There are two different approaches to simplify the modelling of electrons:

- The *jellium* also denoted as *uniform electron gas* or *homogeneous electron gas* model
- The *Fermi gas* model

With both approximations, the exact solution of the Schrödinger equation for electrons in a crystal can be avoided. The jellium is a model for describing the valence electrons in metals and semiconductors mainly applied in solid-state physics. The jellium neglects the atomic or molecular nuclei; however, the model considers the mutual repulsive interactions of electrons. The Fermi gas model even neglects the interaction of electrons. As we consider in this approach only one single valence electron as representative of all electrons in the SiC crystal lattice, we apply the Fermi gas model.

3.2 *Fermi's Golden Rule*

Fermi's golden rule (1950) is based on the work of Dirac (1927) and Wentzel (1927). The rule predicts the transition rate $\lambda_{i\to f}$ from the initial state *i* to the final state *f* under the influence of a weak perturbation relative to a given time interval. The transition rate is the common bridge between quantum physics and reliability engineering. There is

$$\lambda_{i\to f} = \frac{2\pi}{\hbar} \cdot \rho\left(E_f\right) \cdot \left|V_{f,i}\right|^2, \qquad (2)$$

with

- the reduced Planck constant $\hbar \approx 6.582119569\ 10^{-16}$ eV·s,

- the density of states ρ as a function of the final state energy E_f,
- the energy of perturbation V.

4 Predicting the transition rate

The following procedure describes in six steps the approach to predicting the transition rate and the related mean value.

Step 1 Identification of the valence electron quantum numbers
Step 2 Definition of the functional initial state and the faulty final state
Step 3 Calculating the density of states
Step 4 Specification of the perturbation
Step 5 Application of Fermi's golden rule
Step 6 Calculating the mean value

The procedure is exemplarily applied to a silicon carbide (SiC) molecule. Typical SiC semiconductor applications are power electronic devices as Schottky diodes, junction-gate FET, MOSFET, bipolar transistors, and thyristors; moreover, LED or even integrated circuits in space applications. These components are widely involved in safety-related functions as discussed in the framework of functional safety.

4.1 Valence Electrons

Silicon has the electron configuration $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^2$. Hence, the number of electrons is 14 with four valence electrons in the outermost shell, two of them in the 3*s* subshell and the two in the 3*p* subshell.

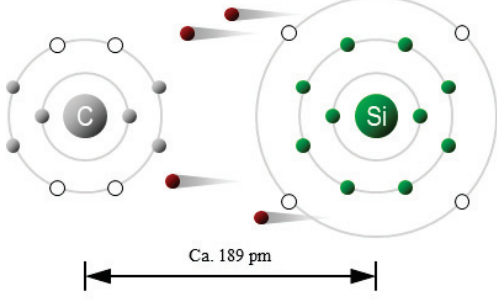

Fig. 1. The simplifying Rutherford–Bohr model (orbits instead of shells) illustrates – rather naively – the journey of the silicon valence electrons into the $n = 2$ orbit of carbon.

The 2*p* subshell of carbon ($1s^2\ 2s^2\ 2p^2$) has four unoccupied places. When silicon and carbon combine to form a silicon carbide molecule, the four silicon valence electrons move into the 2*p* subshell of the carbon atom, see Figure 1. Then the valence electron configuration of silicon carbide is $2p^6$ as the $2s^2$ electrons are non-valent.

Following Step 1 of the procedure given above, the quantum numbers of the valence electrons are identified, see Table 1.

Table 1. Quantum numbers and their denotations of the six SiC valence electrons with the configuration $2p^6$.

Elect. no.	Principal n	Azimuthal ℓ	Magnetic m_l	Spin s
1	2	1	–1	½
2	2	1	0	½
3	2	1	1	½
4	2	1	–1	–½
5	2	1	0	–½
6	2	1	1	–½

4.2 Definition of the Physical and Reliability States

Assumed, a SiC semiconductor is a component of circuit conducting a safety-related function. The obvious failure modes are interruption, short circuit; increase, reduction, or change of specific properties as listed e.g., in IEC 60812:2018.

The root cause may be higher temperature caused internally by the circuit layout or externally. This leads to a damage of the silicon carbide crystalline form. As a consequence, the electrical properties of the component change beyond the specifications of the circuit. The physical component failure leads to a circuit failure and finally to the failure of the safety-related function. This is modelled i.a. in MIL-HDBK-217F, Siemens 29500, IEC 61709:2017, IEC TR 62380:2004 (beloved, misprised, finally replaced), prEN IEC 63142 (project), IEC TR 63162 (project), FIDES Guide 2022.

Defining the physical states, we apply the bra-ket or Dirac notation, respectively, so the definition of the initial state is denoted as vector $|\, i \,\rangle$, which represents the functional state in reliability modelling. We pick out the first electron of Table 1 assigning energy $n = 2$, angular momentum $\ell = 1$, and magnetic property $m_l = -1$ to the initial state vector

$$|\, i \,\rangle = |2, 1, -1\rangle\,. \tag{3}$$

Next, the final state vector $\langle\, f \,|$ is defined, where the electron remains outside the SiC molecule. This represents the faulty state in reliability

modelling. In the physical model, however, the energy level and thus the principal quantum number n of the initial state must be increased so that the electron leaves not only the carbon atom, but the entire SiC molecule. If the number is only increased by one with

$$\langle f| = \langle 3, 0, 0| , \tag{4}$$

the electron might end up in the state of the silicon atom that it had before the molecule was formed. Since the molecule still exists, it would fall back to $|\, i\,\rangle$. As silicon does not have four shells, a two-shell wide ejection starting from $n = 2$ is assumed to be enough to get lost in the conduction band or anywhere else. As we discuss a single electron only, the final state vector is described by

$$\langle f| = \langle 4, 0, 0| . \tag{5}$$

Note that subshell 4*s* offers two places both with $\ell = m_l = 0$, but with two different spins $s = \pm ½$. Then the perturbation V in case of the given reliability application is

$$V_{f,i} = \langle f|\, \nu \,|\, i\rangle, \tag{6}$$

with ν as the incoming photon frequency, see Section 4.4.

4.3 Calculating the density of states

According to Fermi's Golden Rule, the density of states on the energy axis is

$$\rho(E_f) = \frac{\mathrm{d}n}{\mathrm{d}E_f} . \tag{7}$$

It should be noted that ρ is not necessarily the density of *all possible* states in an energy interval, as applied, for example, in solid-state physics. As described above, we assume a fictitious subshell 4*s* of the carbon atom, which is offering just two places of the fourth shell to a hypothetically incoming single electron. With that

$$\rho\big(E_f\big) = 2\ \mathrm{eV}^{-1}. \tag{8}$$

4.4 Specification of the perturbation

Fermi's golden rule gives a quantitative prediction by which an initial state changes into a final state under the influence of a perturbation.

As we are exploring quantum physics here, the first idea would be to consider ionising radiation as perturbation and thus as the root cause of failure. Radiation leads to the photoelectric effect, where an incident photon ejects a valence electron from a molecule. The maximum *kinetic* energy of an ejected electron would be roughly around 1 eV, depending on the material and the frequency of the radiation, e.g., Zinc at 1.2 PHz, which is ultraviolet C, see Table 2, second column.

However, in our approach we discuss perturbations that are well below the photoelectric effect. We consider the range from the thermal region of infrared (long-wavelength IR) around 30 THz to the extreme low frequency of 50 Hz, see Table 2, second column. Although this is a negligible effect in individual cases, due to the fact that SiC is considered to be very robust against radiation, we assume that this will undesirably change the properties of the semiconductor at the atomic level. Since a photon rarely travels alone, this may lead after many incidents, for example, to a semiconductor failure as a component of a space application. With Planck's photo energy equation

$$E(\nu) = \mathrm{h} \cdot \nu , \tag{9}$$

with ν as the frequency of the photon, the energy of a perturbating long-wavelength infrared photon yields E(30 THz) = 0.124 eV. For comparison, an incoming ultraviolet C photon has ca. 5 eV.

4.5 Application of Fermi's golden rule

According to Fermi's golden rule, see equation (2), the transition rate can be defined as a function of the incoming photon frequency ν by

$$\lambda_{i\to f}(\nu) = \frac{2\pi}{\hbar} \cdot 2 \cdot \left| (4\ 0\ 0) \cdot \mathrm{h} \cdot \nu \cdot \begin{pmatrix} 2 \\ 1 \\ -1 \end{pmatrix} \right|^2 \tag{10}$$

4.6 Calculating mean values

With a clear definition of states (see Section 4.2) and given transition rate between these states, the mean time to failure (*MTTF*) can be calculated easily as

$$MTTF = \frac{1}{\lambda_{i\to f}} . \tag{11}$$

Note, the *MTTF* is denoted as *mean operating time to failure* in IEC 60050-192:2015, refer to IEV 192-05-11, or more colloquially as "*mean lifetime*" even assigned to non-biological species. Table 2 lists data for some examples of the electromagnetic spectrum.

Table 2. Extract of an electromagnetic subdivision scheme, refer to Elert (2022), and assigned reliability measures

Denotation	Example Frequency	$\lambda_{i\to f}$ [s^{-1}]	*MTTF* [s]
Ultraviolet C	1.2 PHz	$30 \cdot 10^{+18}$	$33 \cdot 10^{-21}$
IR long-wvl.	30 THz	$19 \cdot 10^{+15}$	$53 \cdot 10^{-18}$
FM radio	100 MHz	$209 \cdot 10^{+3}$	$5 \cdot 10^{-6}$
Super low	25 kHz	$13 \cdot 10^{-3}$	77
Extreme low	50 Hz	$52 \cdot 10^{-9}$	$19 \cdot 10^{+6}$

4.7 Interpretation of results

Although ionising radiation is not considered here as perturbation, the results represent a pretty minimalistic *MTTF*. The values from 10^{-6} down to 10^{-21} seconds can promptly be interpreted as "*immediately* as a photon occurs" in terms of functional safety. Moreover, even low energy electromagnetic waves have an influence on SiC molecules in this model.

The following effect is quite plausible: If the photon frequency increases forty-fold (infrared to ultraviolet), the rate increases by ca. 1500 times.

5 Conclusion

On the one hand, Fermi's golden rule is an established approximation method in quantum physics. On the other hand, the rule offers a very rough modelling as applied here in reliability engineering. However, it would be interesting to see, how semiconductor industry copes with the 2-nanometer technology getting so close to the lattice constants.

Whether conventional computers in semiconductor technology or quantum computers on the rise, the future path of reliability engineering is stepping from installations, assemblies, parts down to molecules, atoms, and electrons.

References

Cheung, R. (2006). *Silicon carbide microelectromechanical systems for harsh environments*. Imperial College Press.

Dirac, P.A.M. (1927). The quantum theory of the emission and absorption of radiation. In: *Proceedings of the Royal Society of London. Series A, Containing Papers of a Mathematical and Physical Character*. Vol. 114, no. 767, March 1927, pp 243–265.

Cui, L.X., Du, Y.-M., and Sun, C. P. (2023), Quantum Reliability. *Physical Review Letters* 131, 160203-1–16203-6.

Elert, Glenn. (Archived from the original on 2022-01-21). The Electromagnetic Spectrum. T*he Physics Hypertextbook*. Retrieved 2024-12-27.

Fermi, E. (1950). *Nuclear Physics*. University of Chicago Press.

Feynman, R., Leighton, R., and Sands, M. (1964). *The Feynman Lectures on Physics. Vol. 3*. California Institute of Technology.

FIDES Group (2022). *FIDES Guide 2022 – Reliability Methodology for Electronic Systems*. FIDES Group, Accra, Ghana.

Giusto, E., Dri, E., Montrucchio, B., Baheri, B., Guan, Q., Tiwari, D., and Rech, P. (2023). Quantum Computing Reliability: Problems, Tools, and Potential Solutions. *53rd Annual IEEE/IFIP International Conference on Dependable Systems and Networks – Supplemental Volume*.

Holmes, M. H. (2013). *Introduction to perturbation methods*, 2nd ed. New York: Springer.

Holzner, St. (2020). *Quantum mechanics for dummies* (in German), 3rd ed. Weinheim, Wiley-VCH.

International Electrotechnical Commission (2018). *Failure modes and effects analysis (FMEA and FMECA)*. IEC 60812:2018-08.

International Electrotechnical Commission (2017). *Electric components – Reliability – Reference conditions for failure rates and stress models for conversion*. IEC 61709:2017-02.

International Electrotechnical Commission (2004). *Reliability data handbook – Universal model for reliability prediction of electronics components, PCBs and equipment*. IEC Technical Report 62380:2004-08, replaced.

International Electrotechnical Commission (2021). *A global methodology for reliability data prediction of electronic components*. IEC 63142:2021-07 Compilation of Comments.

International Electrotechnical Commission (2024). *Electric components – Reliability – Reference failure rates at reference conditions*. IEC Technical Report 63162:2024-02, Draft Technical Report approved.

International Electrotechnical Commission (2015). *International Electrotechnical Vocabulary – Part 192 Dependability*. (IEV 192) IEC 60050-192.

Lin, K., Zhu, J., and Chen, Y. (2020). A non-Hermitian quantum approach to reliability of a two-state system. *Physical Letters A* 384, 1–6.

Park, Y.-S., Willardson, R.K., and Weber E.R. (1998). SiC materials and devices SiC Materials and Devices. 1st Edition, Volume 52. Academic Press.

Safaei, F., Khoddam Astaneh Hossein, M., Sajadi, S. E., and Kouchak Emadi, M. M. (2024) QRP: quantum reliability polynomial for stochastic reliability analysis of reversible circuits. *Quantum Inf Process* 23, 251.

Siemens AG (2004*ff*). *Components, failure rates, expected value*. Part 1–14. SN 29500-1 to 14.

U.S. Department of Defense (1991). *Military Handbook, Reliability Prediction of Electronic Equipment.* MIL-HDBK-217F.

Wentzel, G. (1927). Über strahlungslose Quantensprünge. In: Zeitschrift für Physik. Band 43, Nr. 8, 1927, S. 524–530.

Yazdi, M. (2024) Application of Quantum Computing in Reliability Analysis. In: *Advances in Computational Mathematics for Industrial System Reliability and Maintainability. Springer Series in Reliability Engineering*. Springer, Cham.