Calculation of the Ionisation-Cluster Size Distribution for LEEs in Nanometric Volumes Using A Principle Relevant for Generative Artificial Intelligence

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Notes: 1.) If anything is unclear, you will most likely find it in reference [1].

2.) References are given at the end.

➢ Structure:

1. Motivation

2. Calculation

3. Conclusion

1. Motivation

Awareness raising: Low energy electrons (LEE) refer to a kinetic energy of approx. 100 keV or less.

- **LEEs cause a high degree of single-strand breaks (SSBs) and double-strand breaks (DSBs)**
  → interesting for the development of anticancer drugs and for radiation protection

- **Nanometric volumes are best suited for estimating the action of radiation on biological matter.**

- **Hence, the study of LEEs moving in nanometric volumes is of great interest. However, neither the 'macroscopic' absorbed dose nor the 'microscopic' specific energy are good quantities to describe the action of ionising radiation in nanometric volumes. The observable of choice is the ionisation-cluster size distribution (ICSD).**

➢ Determination of the ionisation-cluster size:

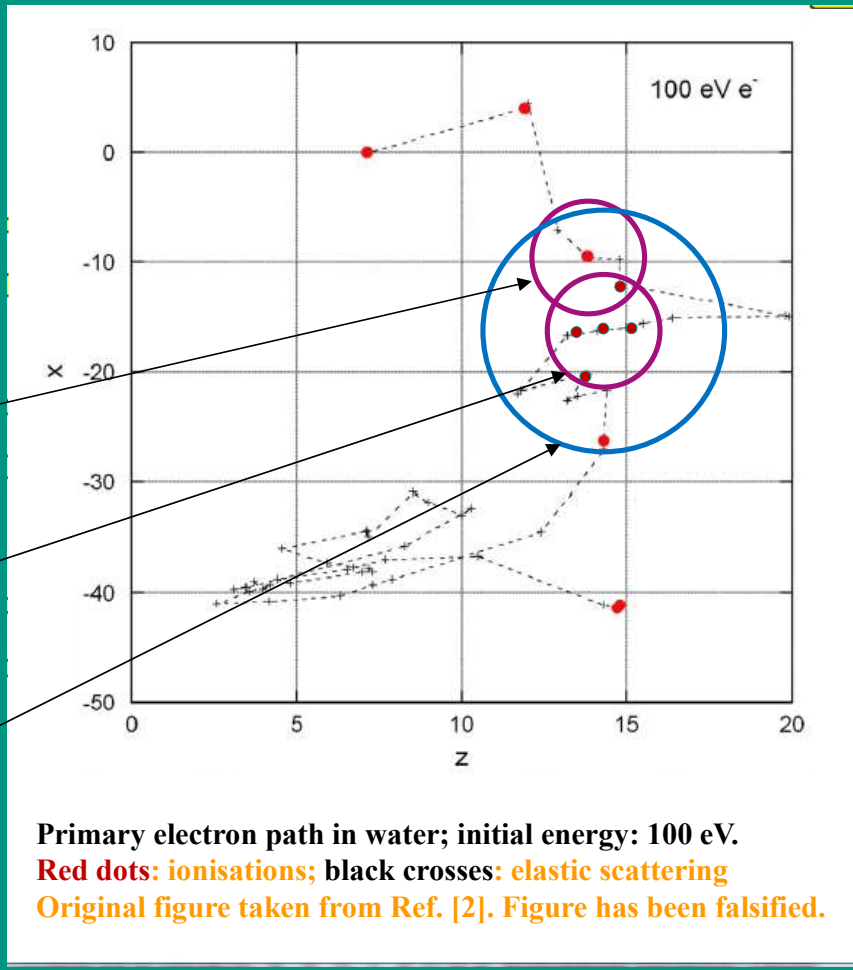
1. Method used to date in this or in a similar form:

One chooses a sphere size to ones taste and places the sphere arbitrarily somewhere (in simple terms). Then, one counts the No of ionisations. That's it.

Sphere/circle with small radius at ionisation 3 contains 2 ionisations.

Sphere/circle with small radius at ionisation 6 contains 5 ionisations.

Sphere/circle with large radius at ionisation 6 contains 7 ionisations.



Primary electron path in water; initial energy: 100 eV.
Red dots: ionisations; black crosses: elastic scattering
Original figure taken from Ref. [2]. Figure has been falsified.

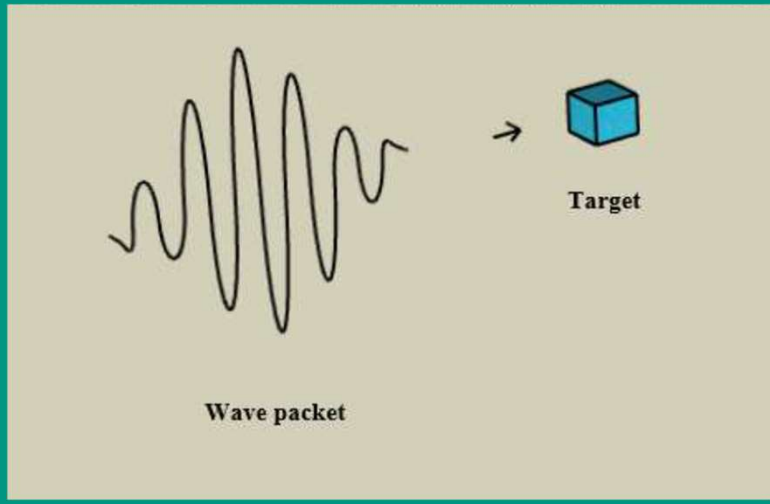
This Method is purely geometric (contains no physics) and the cluster size (i.e. the number of ionisations) depends on the more or less arbitrary assumptions made.

And above all: the method is fundamentally wrong!

Reason: The spatial extension of the wave packet of LEEs is larger than the nanometric target volume itself!

Example: Target volume = 2 x 2 x 2 $(nm)^2$,
E_{kin}(electron) = 100 eV ± 0.4 eV,
Heisenberg's principle ⇒ spatial extension ≈ 60 nm (or more),
i. e. 30 times the cube length!

Approximate illustration →



So,

- **Methods (used so far) based on classical trajectories are fundamentally not suitable for LEEs moving in nanometric volumes.**
- **Quantum mechanical methods are sophisticated and computationally intensive, though.**

My solution/suggestion:

- **Only use trajectory calculations to determine the total No of ionisations (not for the positions), i. e. assume a circumstantial validity of the trajectory method (cf. Ref. [2]).**
- **Use a statistical model for the calculation of the ICSD.**

2. Calculation (using a statistical model)

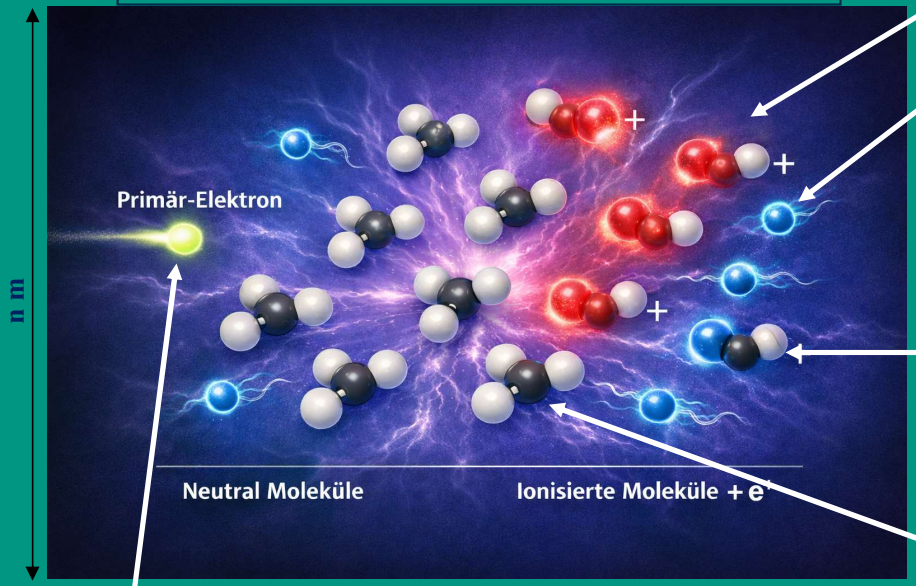
Notation: given a total No of ionisations of 5, $n_t = 5$. These ionisations can result in

– 1 ionisation cluster of size 5:	5	↔ partition vector: $(0, 0, 0, 0, 1)^t$
– 1 ionisation cluster of size 4 and one of size 1:	4 1	↔ partition vector: $(1, 0, 0, 1, 0)^t$
– 1 ionisation cluster of size 3 and one of size 2:	3 2	↔ partition vector: $(0, 1, 1, 0, 0)^t$
– 1 ionisation cluster of size 3 and two of size 1:	3 1 1	↔ partition vector: $(2, 0, 1, 0, 0)^t$
– etc.:	2 2 1	↔ partition vector: $(1, 2, 0, 0, 0)^t$
– etc.:	2 1 1 1	↔ partition vector: $(3, 1, 0, 0, 0)^t$
– etc.:	1 1 1 1 1	↔ partition vector: $(5, 0, 0, 0, 0)^t$

Scenario: - LEEs impinge on a nanometric volume (filled with water or DNA).

- Ionisations and subsequent rearrangement processes (electron hopping, electron attachment, recombination, e. g.) occur, leading to an order-disorder phase transition.

Primary electron hits nanometric volume



Ionised molecule

Electron

Molecule with attached electron

Neutral molecule

Primary electron

Image made by ChatGPT (Feb. 2026, https://chat.openai.com); gives a rough idea only

Electron hopping

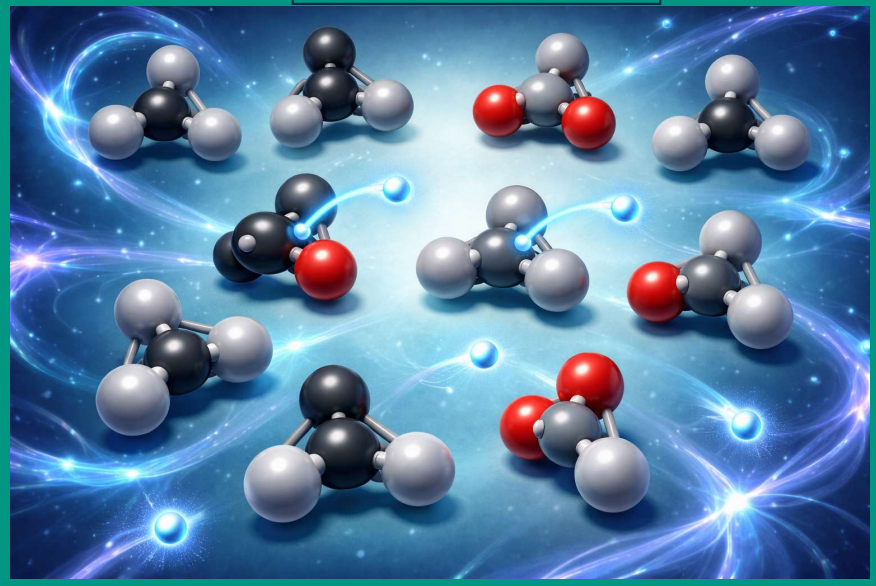


Image made by ChatGPT (Feb. 2026, https://chat.openai.com); gives a rough idea only

Assumption: The statistical ensemble of imaginary uniform ionisation-cluster systems is a canonical one.

Basic idea:

Do for all events:

(A) calculate all possible partitions of the number n_t of ionisation interactions,

(B) calculate the temperature T and the free energy F, and

(C) choose a set of partitions which refers to n_t ionisations and M ionisation clusters due to "exp{-F((n_t, M), T, V)/T}" as well as select a microstate with equal probability then.

Remarks:

Regarding "(A): calculate all possible partitions of the number of ionisation interactions":

If $n_t = 10$, then the No of partitions is 42.
If $n_t = 100$, then the No of partitions is 190 569 292.
If $n_t = 1000$, then the No of partitions is 24 061 467 864 032 622 473 692 149 727 991.
The calculation of all possible partitions is a so-called NP-complete decision problem.

Fortunately, $n_t < 100$ for LEEs in nanometric volumes; calculation is very quick --- it feels 'instant'.

(For larger mesoscopic systems, one can proceed as mentioned in Ref. [1]. Furthermore, it is possible to store and compute partitions using quantum registers and quantum gates. So a computer could be used in the future whose central processing unit has been expanded to include a quantum processing unit.)

Regarding "(B): calculate the temperature T and the free energy F":

First, the temperature is calculated by,

$$E_{abs} = \frac{3\,e^2 n_t^2}{20\,\pi\varepsilon_0\,R} + \sum_{j=1}^{n_t} n_j\,[F_j(T,V) - T\,(\frac{\partial F_j(T,V)}{\partial T})_V] - E_0.$$

Absorbed energy — Coulomb energy — Internal energy — Ground-state energy

Result:

$$T = \Theta_1 E_{abs} - \Theta_2\,.$$

There is no chicken-and-egg problem with respect to F and T, since the information contained in F is also contained in the absorbed energy!

$$\Theta_1 = \left[\frac{3}{2}\,k_B\left(\sum_{j=1}^{n_t} n_j^2 - n_t\right)\right]^{-1}$$

$$\Theta_2 = \Theta_1 \frac{3\,e^2}{20\,\pi\,\varepsilon_0\,R}\left(n_t^2 + \sum_{j=1}^{n_t}\left(\frac{R}{\tilde{r}_k} + n_j^2\right) j^2 n_j\right)$$

Then, the free energy is calculated by,

$$F((n_t, M), T, V) = \sum_{j=1}^{n_t} (F_j^{tr,Z} + n_j F_j^{in})$$

Translational parts — Inner parts

$$F_j^{tr,Z} = -k_B T \ln Z(T, n_j, V)$$

$$Z(\mathrm{T}, n_j, \mathrm{V}) = \frac{\lambda_T^{-3n_j}}{n_j!} \int e^{-\beta V_m(\vec{x})}\, d^{3n_j}x$$

$$Z(\mathrm{T}, n_j, \mathrm{V}) = \frac{\lambda_T^{-3n_j}}{n_j!} (C_1 C_2 e^{-\beta H_1})^{n_j}$$

$$V_m(\vec{x}) = V_m'(\vec{x_1}) + \cdots + V_m'(\vec{x_{n_j}})$$

$$V_m'(\vec{x}_i) = V_m'(x_i) = \frac{e^2 j(n_t - j)}{8\pi\varepsilon_0 R}\left(3 - \frac{x_i^2}{R^2}\right)$$

Coulomb energy of a cluster of size "j" at position "$\vec{x}_i$"

dependant on "erfi", because of

$$\mathrm{F_j^{in}} = \frac{1}{4\pi\varepsilon_0}\,\frac{3}{5}\,\frac{e^2 j^2}{\tilde{r}_k}$$

Regarding "(C): choose a set of partitions which refers to n_t ionisations and M ionisation clusters due to "exp{-F((n_t, M), T, V)/T}" as well as select a microstate with equal probability then":

- **Entropy is contained in the argument of the exponential function. So the principle of selection can be rewritten to a principle of selection with maximum entropy!**

- **Maximum entropy principle is well know in physics. Using Shannon information, one can calculate Shannon entropy "H_S" and apply the principle of maximum (minimum) entropy in generative AI. Example regarding H_S: Sampling of words in large language models.**

➢ **Note:**

One can calculate Shannon information and Shannon entropy "H_S" for each partition. And it is possible to convert "H_S" into the statistical thermodynamic entropy "S_t":

$$S_t = H_S \, \mathrm{k} \ln 2.$$

Boltzmann constant

However, the conversion, i.e. the physical embedding, requires assumptions (restrictions) and is extremely complicated!

3. Conclusion

- The determination of the ionisation-cluster sizes for LEEs moving in nanometric volumes cannot be carried out using methods based on trajectories, as the spatial extension of the electrons is much greater than the volume itself.
- Quantum mechanical methods are too complex.
- Suggested solution: use a statistical thermodynamic model and generate the ICSD using a principle analogous to the maximum-entropy principle.
- How successful the model is remains to be seen!

Thank you very much for your attention!

➢ References:

[1] Heide, B.: Proposal on the Calculation …, arXiv:2404.03961.

[2] Liljequist, D. and Nikjoo, H.: On the validity of trajectory ..., Radiation Physics and Chemistry 99 (2014) 45-52.