2nd Asia-Pacific Conference on Plasma Physics, 12-17,11.2018, Kanazawa, Japan

Modelling plasmas and liquids: including electron solvation as a non-equilibrium process

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A complete model of plasmas impacting on liquids and soft-tissues requires an understanding of microscopic transport of electrons and ions throughout liquids. In gases, the transport of electrons is well understood. swarm transport simulations can track individual charged particles as they move through a neutral gas or liquid, predicting transport quantities such as drift velocities, ionisation coefficients and lifetimes. State of the art codes for both Monte Carlo simulation and Boltzmann equation solution of transport in gases have proven their high accuracy and are now as good as their inputs [1].

In contrast, liquids or even dense gases present many features [1-3] that make the life of a modeller difficult:

a. the electron is a "quasi-free" particle, as it is never far from any neutral particle
b. scattering from a single neutral is always "screened" by the surrounding neutrals
c. the medium has short-range but no long-range order, precluding a solid-state approach
d. the medium can respond to the e^- giving rise to self-trapping.

In this presentation, I will focus on the last point, showing how we can model the trapping of an electron in a liquid using an ab-initio non-equilibrium model. Self-trapping in a liquid is more commonly known as "solvation".

The model provides two quantities that can be directly used in simulations: a solvation cross section and a residence time distribution. These quantities are functions of the electron energy, allowing for a completely non-equilibrium description of the solvation. Importantly, these quantities are required for a kinetic theory model of electron solvation.

I will also show how the ab initio model can provide useful information such as:

- Solvation timescales.
- Influence of external and self-consistent fields.
- How "aborted" solvation affects quasi-free transport.
- The interaction of solvation with other species in the plasma.

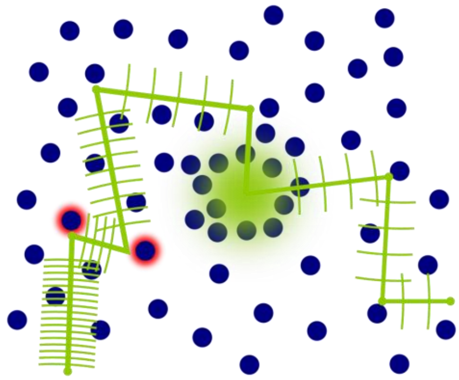

Figure 1 – the path of a light particle in a liquid is dominated by its quantum nature. Shown in the centre is a (temporary) self-trapping of the light particle by a density fluctuation.

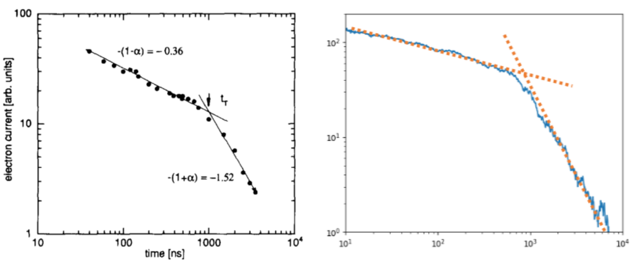

Fig. 14. Scher–Montroll plot of the data of fig. 10c.

Figure 2 – a comparison of experimental measurement (left, from [4]) with theoretical simulations (right) for electron propagation in liquid neon. Fractional transport [5] and Scher-Montroll-like behavior is observed due to the temporary localization (solvation) in the liquid.

References:

[1] White et al, PSST **27** 053001 (2018)
[2] Boyle et al, J Chem Phys **142** 154507 (2015)
[3] Boyle et al, PSST **26** 024007 (2017)
[4] Sakai et al, Chem. Phys. **164** 139 (1992)
[5] Philippa et al Phys. Rev. E **84** 041138 (2011)