Single-or double-electron emission within the Keldysh nonequilibrium Green's function – a diagrammatic approach

Yaroslav Pavlyukh*,†, Michael Schüler†[1], Jamal Berakdar†

* Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, D-67653 Kaiserslautern, Germany

† Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany

Synopsis We extend the general theory of electron and double electron photoemission from correlated systems based on the nonequilibrium Green's functions approach. The theory can be applied to a range of processes in interaction many-body systems, including plasmonic losses due electron-plasmon coupling during the photoemission process. As an application, we study the plasmon-mediated double photoemission from the C_{60} molecule.

In full generality, photoemission is a complicated process, where a variety of effects can occur during the ionization process. This includes, for instance, resonant states, plasmon satellites or the simultaneous emission of two electrons – the (non-sequential) double photoelectron emission or double photoemission (DPE).

Following the transition from molecules towards solids, the effective electron-electron (e–e) interaction is determined, besides the Coulomb repulsion, by the charge-density fluctuations of the dynamical environment – this where DPE comes into play as a powerful spectroscopy to access the e–e interaction directly.

For solid-state systems, the Green's function formalism has been established as the most versatile approach to incorporate electronic excitations and other interaction effects, such as electron-plasmon or electron-phonon coupling. In order describe photoemission or DPE from larger molecules or solids, a Green's function formulation is highly desirable. In this contribution, we present a systematic route for constructing Feynman diagrams for DPE which can account for all these many-body effects [1].

The theory is applied to DPE from the C_{60} molecules. The pronounced plasmonic excitations [2] give rise to a strong, dynamically screened e–e interaction which is identified as the central driving force of the process of plasmons-mediated DPE. Within this process, the inelastic scattering of an emanating photoelectron induces collective modes, which then decay upon emitting a second electron. We analyze this mechanism in detail, corroborate the findings by model and by first-principle calculations and compare to experiments (see Fig. 1).

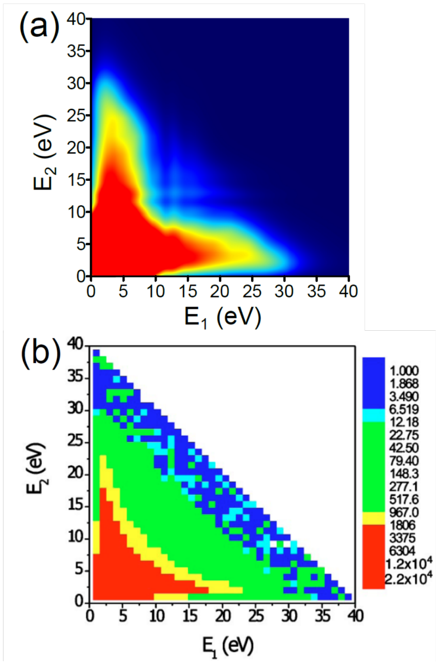

Figure 1. Comparison of the DPE cross-section as function of the energy E_1, E_2 of each of the two photoelectrons (a) our calculation, and (b) experimental results by Hillebrecht *et al.* [3].

References

[1] Y. Pavlyukh, M. Schüler, J. Berakdar 2015 *Phys. Rev. B* **91** 155116

[2] M. Schüler, J. Berakdar, Y. Pavlyukh 2015 *Phys. Rev. A* **92** 021403(R)

[3] F. U. Hillebrecht *et al.* 2005 *Phys. Rev. B* **71** 125406

[1]E-mail: michael.schueler@physik.uni-halle.de