Feynman diagrams in the new era of super-computers. Is the gap between theory and computation any smaller?

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Abstract

The development of computer codes (http://psi-k.net/software/) and platforms (http://www.aiida.net/) to allow massive material science calculations have, in the last twenty years, changed the way condensed and molecular physics calculations are actually performed. And have also created a gap between theory and computation.

A new area of applied physics boosted and, moving the steps from the ab-initio community, exploded in the novel *Material Science community*. In practice this transition was accompanied by a huge increase of efforts in porting scientific codes (developed by physicists) to High Performance Computers (developed by technicians). With the net results that many physicists turned into…technicians.

Despite this could appear as a detriment of theoretical condensed and molecular physics the plan of this talk is to demonstrate that this not actually the case. After a first period where, as expected, most of the development has been to export to HPC's (High Performance Computers) existing tools now we can have a new era where theoretical models can be directly and (more or less) quickly tested against experiments. The short bridge created by the development of tools for the material science community via the use of HPCs can potentially allow calculations of phenomena whose description was just impossible few years ago.

In this talk a will give a very personal description of the way the codes have changed the scenario of applied theoretical physics and, more importantly, how the future looks like. I will discuss two examples in the field of ultra-fast phenomena: exciton (bound electron-hole pair) real-time formation and combined atomic/electronic dynamics on the attosecond time-scale.