Early Days of CC Theory and a Glimpse in the Future

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The primary intent of my talk is to recall early days of CC theory, its roots in the MBPT and initial attempts of its implementation in nuclear physics, culminating in Jiří Čížek's pioneering work formulating explicit CC equations that are germane to the many-electron correlation problem – the work whose 50th anniversary this Symposium celebrates. I will also mention our initial joint efforts in actual exploitation of the CC formalism at both the semi-empirical and ab initio levels. The former one considered the PPP and Hubbard cyclic polyene model – a notoriously difficult problem still extant today – which led us to investigate Hartree-Fock stability problems. The latter one, addressing primarily the role of triples, was much more successful and promising.

The subsequent developments led to multifarious exploitations of CC methodology and will be undoubtedly documented in subsequent talks. Yet, in spite of the successes of the single-reference CCSD, and especially its CCSD(T) version perturbatively corrected for triples, the presence of quasi-degeneracy when breaking chemical bonds or dealing with strongly correlated systems continues to represent a challenge. One possible avenue to overcome these problems led to the so-called externally and internally corrected CCSD approaches. Since the latter ones recently enjoyed a certain renaissance, I will try to interrelate these developments and highlight advances made in this direction.

Finally, time permitting, I will try to speculate if our half-a-century lasting efforts might one day be supplanted by quantum computers.