A Quantum Chemistry Perspective on Many-Body Electronic Structure Methods

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In recent years, many-body electronic structure methods have been successfully transferred between theoretical condensed matter physics and quantum chemistry, fostering a growing interest in understanding the connections between these approaches.
In this talk, I will present a rigorous connection between the G_0W_0 method and the equation-of-motion coupled-cluster (EOM-CC) approach for charged excitations [1, 2]. Building on this connection, I will show how analytic nuclear gradients can be derived for both G_0W_0 and the Bethe–Salpeter equation (BSE) within a GW-based framework [3, 4]. Finally, to address the computational cost of many-body methods, I will discuss a newly developed library implementing tensor hypercontraction techniques for the electron repulsion integrals [5].

References

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