Current status and challenges of explicitly correlated electronic structure theory

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Since an r_{12}-dependent wavefunction was first employed by Hylleraas for the He atom [1], numerous attempts have been made for constructing practical explicitly correlated methods, e.g. correlated Gaussian and transcorrelated approaches. F12 theory established in the 2000s which inherits the R12 technology [2, 3] arguably provides the most accurate and efficient ansatz exploiting the cusp conditions (SP-ansatz) in conjunction with the short-range exponential (Slater-type) correlation factor. Rapid progress of F12 has significantly extended the application range of explicitly correlated theory, offering potential wavefunction treatments of complex systems [4]. My talk will survey explicitly correlated electronic structure approaches and indicate some future challenges.

References

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