Towards a bound-state relativistic QED approach

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Atomic and molecular few-particle bound states are of interest in both experimental and theoretical precision spectroscopy. In combination with theoretical computations, the experiments are proposed to test our fundamental understanding of ordinary matter in the low-energy range and to probe physics beyond the Standard Model. Relativistic and QED effects are most often treated within the non-relativistic quantum electrodynamics framework, which yields excellent agreement with experimentally measured transitions for low-Z systems (e.g., [1]). Nevertheless the large number of effective interaction terms makes evaluating higher-order corrections increasingly complicated both analytically and numerically. In this contribution, the development of an alternative approach based on the relativistic Bethe–Salpeter wave equation is presented for the simplest two-fermion case. The introduction of the equal-time wave function and separating a non-retarded interaction kernel gives rise to the no-pair Dirac–Coulomb(–Breit) equation, which is solved variationally to high precision using an explicitly correlated Gaussian basis set, treating both relativistic and correlation 'effects' on an equal footing [2, 3, 4, 5, 6]. The method is applied to several two-electron atomic and molecular systems with clamped nuclei, and further extended to pure two-body systems without the Born–Oppenheimer approximation such as positronium, muonium, hydrogen atom, and muonic hydrogen [7]. The numerical results show excellent agreement with the corresponding relativistic perturbative energy contributions. Challenges and advances towards the inclusion of higher-order pair, retardation, and radiative contributions are discussed [8].

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