A static quantum embedding scheme based on coupled cluster theory

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We have developed a static quantum embedding scheme based on the projection equations to solve coupled-cluster amplitudes. In the spirit of other quantum embedding methods, we solve the local fragment problem with a higher-level method and the environment problem with a low-level method, thereby keeping the computational complexity low. We solve the environment and the fragment problem self-consistently so that the fragment coupled cluster amplitudes can capture all the environmental effects. The interaction term for the fragment problem in this method is renormalized by the quantities from a low-level method. We have investigated the current method with a few prototypical molecular examples to show that we reach comparable accuracy to what would be achieved by applying the high-level method for the entire system. Furthermore, we show that it is possible to systematically improve the accuracy of the observables by increasing the fragment size. Also, this method does not show any artefact with the increase of basis set size, which is essential to systematically improve our results.