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Embedding four-body correlation into antisymmetrized geminal power wave function AIRI KAWASAKI, OSAMU SUGINO, The Institute for Solid State Physics, University of Tokyo — We extend the Coleman's antisymmetrized geminal power (AGP) to develop a variational wave function theory that can incorporate up to four-body correlation in a region of strong correlation. AGP has been used in the variational Monte Carlo (VMC) simulation by multiplying a Jastrow-type correlation factor, but here we develop a formalism to deterministically obtain the total energy and its derivatives in order to avoid the statistical fluctuation that hampers evaluation of the atomic force for geometry optimization and molecular dynamics simulation. For this purpose, we developed a total energy formula in terms of the traces of geminal powers. This novel trace formula is applied to a simple Hubbard ring model to test its numerical accuracy and robustness. The result shows a promising step toward development of a first-principles wave function theory for a strongly correlated point defect or adsorbate embedded in an AGP-based mean-field medium.

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