Monte Carlo Study of the Exchange-Correlation Energy Density in Atomic Silicon

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The Coulomb-coupling constant integration technique is used with variational quantum Monte Carlo (VQMC) to study different approximation methods within spin density functional theory. By using VQMC, realistic many-body ground state trial wave functions are generated for the spin-polarized silicon pseudo atom at different values of the Coulomb coupling constant. Through these wavefunctions, the ground state ensemble averaged charge densities, pair-correlation function, exchange-correlation hole, and exchange-correlation energy density are found. The exchange-correlation energy density is expressed via the spherically averaged exchange-correlation hole and compared to the results generated from the local spin density approximation (LSDA), a spin dependent generalized gradient approximation (GGA), a new version of the weighted spin density approximation, and the average density approximation. Through this methodology, the limits of the LSDA and GGA are seen, and why particular non-local approximations generate better results for the exchange-correlation energy density for spin-polarized systems of valence electrons is discussed.