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Optimizing Fermion Nodes With Diffusion Monte Carlo and Gradient Descent JOHN MCFARLAND, EFSTRATIOS MANOUSAKIS, Florida State University — We present a method for optimizing the fermion ground state nodes using only diffusion Monte Carlo (DMC) with gradient descent. The method iteratively shifts the parameters of an arbitrary node-fixing trial function in the opposite direction of the DMC energy gradient. The energy gradient is calculated from DMC walker distributions by one of three methods we derive from an analytical expression. We combine our gradient calculation methods with various gradient descent algorithms and apply these "training" algorithms to trial functions of Be, Li_2, and Ne, all consisting of a single Slater determinant with randomized parameters. This dramatically improves the nodes to the same level as those optimized by variational Monte Carlo. Our method therefore enables DMC to be independent, departing from the standard procedure of optimizing the nodes with a non-DMC scheme such as variational Monte Carlo, Density function theory, or configuration interaction based calculation, which do not directly minimize the DMC energy.

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