qflow documenation

JN

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1 Terminology

VMC simulation - A complete VMC simulation using

2 qflow.training

qflow.training.train(***psi, H, sampler, iters, samples, gamma, optimizer, verbose, call_backs, call_back_resolution*** **)**

1. psi - Wavefunction class from qflow.wavefunctions
2. H - Hamiltonian class from qflow.hamiltonians
3. sampler - Sampler class from qflow.samplers
4. iters - Number of complete VMC simulations used during training
5. samples -
6. gamma -
7. optimizer -
8. verbose -
9. call_backs -
10. call_back_resolution -

3 qflow.Hamiltonian

qflow.Hamiltonian.optimize_wavefunction(***psi, sampler, iterations, samples, optimizer, gamma, verbose*** **)**

1. psi - Wavefunction class from qflow.wavefunctions
2. sampler - Sampler class from qflow.samplers
3. iterations - Number of complete VMC simulations used during training
4. samples -
5. optimizer -
6. gamma -
7. verbose -

optimize_wavefunction uses a 0.2 burn-in ratio to the total samples in each iteration.