

December 1, 2025

1 VQE Benchmark Suite for Lithium Hydride (LiH) - Frozen Core Version (8 Qubits)

This notebook implements a **comprehensive benchmark framework** to compare multiple ansatz implementations for VQE.

Framework Features: - Tests 4 different ansatz implementations - Runs each ansatz 3 times for statistical reliability - Tracks comprehensive metrics for each run - Aggregates results into comparison tables and visualizations

Ansätze to Compare: 1. **UCCSD** - Unitary Coupled Cluster Singles and Doubles 2. **Hardware Efficient** - Parameterized rotation layers 3. **TwoLocal** - General two-local ansatz 4. **Custom Ansatz** - To be implemented

Metrics Tracked: - Circuit complexity (CNOT count, depth, parameters) - Convergence speed and quality - State fidelity to exact ground state - Variance behavior - Barren plateau indicators

```
[9]: # Install required packages
!pip install --upgrade qiskit qiskit-nature qiskit-algorithms pyscf matplotlib
    ↵-q
```

[notice] A new release of pip is available: 24.0 → 25.3
[notice] To update, run:
pip install --upgrade pip

```
[10]: # Import required libraries
from qiskit_nature.units import DistanceUnit
from qiskit_nature.second_q.drivers import PySCFDriver
from qiskit_nature.second_q.transformers import FreezeCoreTransformer
from qiskit_nature.second_q.mappers import JordanWignerMapper
from qiskit_nature.second_q.circuit.library import HartreeFock, UCCSD, UCC
from qiskit.circuit.library import ExcitationPreserving
from qiskit.circuit.library import TwoLocal, EfficientSU2
from qiskit_algorithms import VQE, NumPyMinimumEigensolver
from qiskit_algorithms.optimizers import SPSA, COBYLA, L_BFGS_B
from qiskit_primitives import StatevectorEstimator
from qiskit_quantum_info import Statevector, state_fidelity
```

```

import matplotlib.pyplot as plt
import numpy as np
import pandas as pd
import time
from typing import Dict, List, Any

print(" All libraries imported successfully!")

```

All libraries imported successfully!

1.1 Step 1: Define LiH Molecule with Frozen Core

```
[11]: # Define LiH molecule
driver = PySCFDriver(
    atom="Li 0 0 0; H 0 0 1.595",
    basis="sto3g",
    charge=0,
    spin=0,
    unit=DistanceUnit.ANGSTROM,
)

# Run electronic structure calculation
problem_full = driver.run()

print(f"Before freeze-core:")
print(f"  Spatial orbitals: {problem_full.num_spatial_orbitals}")
print(f"  Particles: {problem_full.num_particles}")
print(f"  Qubits: {problem_full.num_spatial_orbitals * 2}\n")

# Apply frozen core approximation
transformer = FreezeCoreTransformer(
    freeze_core=True,
    #remove_orbitals=[4, 5]
    remove_orbitals=[5] # Remove 2 high-energy orbitals: 6-4 spatial orbitals
)
problem = transformer.transform(problem_full)

print(f"After freeze-core:")
print(f"  Spatial orbitals: {problem.num_spatial_orbitals}")
print(f"  Particles: {problem.num_particles}")
print(f"  Qubits: {problem.num_spatial_orbitals * 2} (Target: 8)")
print(f"  Nuclear repulsion: {problem.nuclear_repulsion_energy:.6f} Ha")
```

Before freeze-core:

Spatial orbitals: 6
 Particles: (2, 2)
 Qubits: 12

```

After freeze-core:
  Spatial orbitals: 4
  Particles:        (1, 1)
  Qubits:          8 (Target: 8)
  Nuclear repulsion: 0.995318 Ha

```

1.2 Step 2: Get Hamiltonian and Map to Qubits

```
[12]: # Get Hamiltonian from reduced problem
hamiltonian = problem.hamiltonian
second_q_op = hamiltonian.second_q_op()

# Map to qubit operator
mapper = JordanWignerMapper()
qubit_op = mapper.map(second_q_op)

print(f"Fermionic operator has {len(second_q_op)} terms")
print(f"Qubit operator has {len(qubit_op)} terms")
print(f"Number of qubits: {qubit_op.num_qubits}")

```

```

Fermionic operator has 300 terms
Qubit operator has 105 terms
Number of qubits: 8

```

```

Qubit operator has 105 terms
Number of qubits: 8

```

1.3 Step 3: Exact Solution (NumPy Solver)

```
[13]: # Exact solver for reference
numpy_solver = NumPyMinimumEigensolver()
numpy_result = numpy_solver.compute_minimum_eigenvalue(qubit_op)

exact_electronic = numpy_result.eigenvalue.real
exact_total = exact_electronic + problem.nuclear_repulsion_energy

# Get exact ground state vector for fidelity calculation
exact_state = numpy_result.eigenstate

print("Exact Solution (NumPy):")
print(f"  Electronic energy: {exact_electronic:.8f} Ha")
print(f"  Total energy:      {exact_total:.8f} Ha")

```

```

Exact Solution (NumPy):
  Electronic energy: -1.06086814 Ha
  Total energy:      -0.06555051 Ha

```

1.4 Step 4: Define Benchmark Framework and Ansatz Configurations

```
[14]: def run_vqe_benchmark(ansatz, ansatz_name, run_number, qubit_op, ↴exact_electronic, exact_state, problem, maxiter=300):
    """
    Run a single VQE benchmark with comprehensive metric tracking
    FIXED: Robust error handling in callback
    """
    decomp_ansatz = ansatz.decompose()

    num_parameters = decomp_ansatz.num_parameters
    circuit_depth = decomp_ansatz.depth()
    circuit_size = decomp_ansatz.size()
    cnot_count = decomp_ansatz.count_ops().get('cx', 0)

    # # ##debug checks below ----##
    # # Test params
    # test_params = np.random.normal(0, 0.1, size=num_parameters)
    # param_dict = {param: test_params[i] for i, param in enumerate(ansatz.
    ↴parameters)}
    # bound_circuit = ansatz.assign_parameters(param_dict)

    # # Check before decompose
    # print(f"    Before decompose:")
    # print(f"        Depth: {bound_circuit.depth()}")
    # print(f"        Gates: {bound_circuit.size()}")
    # print(f"        Ops: {bound_circuit.count_ops()}")

    # # Check after decompose
    # decomposed = bound_circuit.decompose()
    # print(f"    After decompose:")
    # print(f"        Depth: {decomposed.depth()}")
    # print(f"        Gates: {decomposed.size()}")
    # print(f"        Ops: {decomposed.count_ops()}")
    # #---#####

    print(f"\n{'='*70}")
    print(f"Running: {ansatz_name} - Run #{run_number}")
    print(f"Optimizer: COBYLA (maxiter={maxiter})")
    print(f"Parameters: {num_parameters}, Depth: {circuit_depth}")
    print(f"{'='*70}")

    start_time = time.time() #moved here now
```

```

# Initialize tracking lists
convergence_history = []
all_evaluations = []
variance_history = []

best_energy = [float('inf')]
callback_error_count = [0]

def callback(eval_count, parameters, mean, std):
    """Callback with robust error handling"""
    try:
        # Store all evaluations
        all_evaluations.append(mean)

        # Update best-so-far
        if mean < best_energy[0]:
            best_energy[0] = mean

        # Store best-so-far for convergence
        convergence_history.append(best_energy[0])

        # Extract variance (simplified - don't let this fail)
        try:
            if isinstance(std, dict):
                variance_val = list(std.values())[0] if len(std) > 0 else 0.
            else:
                variance_val = std if std is not None else 0.0
            variance_history.append(variance_val)
        except:
            variance_history.append(0.0)

        # Print progress every 50 evaluations
        # if len(all_evaluations) % 50 == 0:
        #     print(f"Eval {len(all_evaluations)}: E={mean:.6f} Ha, " +
        #           f"Error={abs(mean - exact_electronic)*1000:.3f} mHa")

        #print every eval:
        print(f"Eval {len(all_evaluations)}: E={mean:.6f} Ha, " +
              f"Error={abs(mean - exact_electronic)*1000:.3f} mHa")

    except Exception as e:
        # Count errors but don't let callback crash VQE
        callback_error_count[0] += 1
        if callback_error_count[0] == 1: # Only print first error
            print(f"Callback error: {e}")

```

```

# Run VQE with COBYLA optimizer
vqe_solver = VQE(
    StatevectorEstimator(),
    ansatz,
    COBYLA(maxiter=maxiter, tol=1e-6),
    callback=callback
)

# Use small random initialization to avoid symmetry/barren plateaus
np.random.seed(42 + run_number) # Different seed per run
vqe_solver.initial_point = np.random.normal(0, 0.01, size=num_parameters)

print(f"  Starting VQE optimization now...") # debug
vqe_start = time.time() # debug

result = vqe_solver.compute_minimum_eigenvalue(qubit_op)

vqe_end = time.time() # debug
print(f"  VQE compute_minimum_eigenvalue took: {vqe_end - vqe_start:.1f}s") # debug

vqe_electronic = result.eigenvalue.real
vqe_total = vqe_electronic + problem.nuclear_repulsion_energy
elapsed_time = time.time() - start_time

# Get actual number of function evaluations
actual_evals = getattr(result.optimizer_result, 'nfev', len(convergence_history))

print(f"\n  Completed in {elapsed_time:.1f}s")
print(f"  Function evaluations: {actual_evals}")
print(f"  Callback captured: {len(convergence_history)} points")
if callback_error_count[0] > 0:
    print(f"  Callback errors: {callback_error_count[0]}")

# Calculate convergence speed
if len(convergence_history) > 1:
    energy_range = convergence_history[0] - exact_electronic
    threshold_energy = convergence_history[0] - 0.99 * energy_range
    convergence_iter = next((i for i, e in enumerate(convergence_history)
                             if e <= threshold_energy), len(convergence_history))
else:
    convergence_iter = actual_evals

# Calculate final state fidelity

```

```

try:
    optimal_params = result.optimal_parameters
    if optimal_params is not None:
        param_dict = {param: optimal_params[param] for param in ansatz.
        ↪parameters}
        bound_circuit = ansatz.assign_parameters(param_dict)
    else:
        bound_circuit = ansatz.assign_parameters(vqe_solver.initial_point)

    final_vqe_state = Statevector(bound_circuit)
    final_fidelity = state_fidelity(final_vqe_state, exact_state)
except Exception as e:
    print(f"      Fidelity calculation failed: {e}")
    final_fidelity = 0.0

# Calculate final metrics
final_energy_error = abs(vqe_electronic - exact_electronic)
final_energy_error_percent = (final_energy_error / abs(exact_electronic)) * ↪
    ↪100

    print(f"      Energy Error: {final_energy_error:.6e} Ha"
    ↪({final_energy_error_percent:.4f}%)")
    print(f"      Fidelity: {final_fidelity:.6f}")
    print(f"      Convergence: {convergence_iter}/{len(convergence_history)}"
    ↪iterations")

# Plot convergence on second run (only if we have data)
if run_number == 2 and len(convergence_history) > 1:
    print(f"\n{'*'*70}")
    print(f"  PLOTTING CONVERGENCE FOR {ansatz_name} - RUN #2")
    print(f"{'*'*70}\n")

    fig, (ax1, ax2) = plt.subplots(1, 2, figsize=(14, 5))
    iterations = range(1, len(convergence_history) + 1)

    # Plot 1: Energy convergence
    ax1.plot(iterations, convergence_history, 'b-', linewidth=2, alpha=0.7,
    ↪label='VQE Energy')
    ax1.axhline(y=exact_electronic, color='r', linestyle='--', linewidth=2,
    ↪label='Exact Energy')
    ax1.set_xlabel('Iteration', fontsize=12)
    ax1.set_ylabel('Electronic Energy (Ha)', fontsize=12)
    ax1.set_title(f'{ansatz_name} - Energy Convergence (Run #2)',
    ↪fontsize=13, fontweight='bold')
    ax1.legend(fontsize=10)
    ax1.grid(True, alpha=0.3)

```

```

# Plot 2: Absolute error (log scale)
absolute_errors = [abs(energy - exact_electronic) for energy in convergence_history]
ax2.semilogy(iterations, absolute_errors, 'g-', linewidth=2, alpha=0.7)
ax2.set_xlabel('Iteration', fontsize=12)
ax2.set_ylabel('Absolute Energy Error (Ha)', fontsize=12)
ax2.set_title(f'{ansatz_name} - Error Convergence (Run #2)', fontsize=13, fontweight='bold')
ax2.grid(True, alpha=0.3, which='both')

plt.tight_layout()
plot_filename = f"convergence_{ansatz_name}_run2.png"
plt.savefig(plot_filename, dpi=150, bbox_inches='tight')
plt.show()
print(f" Convergence plot saved: {plot_filename}\n")

# Return comprehensive results
return {
    'Ansatz': ansatz_name,
    'Run': run_number,
    'CNOT_Count': cnot_count,
    'Circuit_Depth': circuit_depth,
    'Circuit_Size': circuit_size,
    'Num_Parameters': num_parameters,
    'Total_Iterations': len(convergence_history) if len(convergence_history) > 0 else actual_evals,
    'Convergence_Speed_99': convergence_iter,
    'Total_Time_sec': elapsed_time,
    'Initial_Energy_Ha': convergence_history[0] if len(convergence_history) > 0 else vqe_electronic,
    'Final_Energy_Ha': convergence_history[-1] if len(convergence_history) > 0 else vqe_electronic,
    'Exact_Energy_Ha': exact_electronic,
    'Energy_Error_Ha': final_energy_error,
    'Energy_Error_Percent': final_energy_error_percent,
    'State_Fidelity': final_fidelity,
    'Fidelity_Percent': final_fidelity * 100,
    'Avg_Variance': np.mean(variance_history) if len(variance_history) > 0 else 0.0,
    'Final_Variance': np.mean(variance_history[-100:]) if len(variance_history) > 100 else 0.0,
    'Max_Variance': max(variance_history) if len(variance_history) > 0 else 0.0,
    'Min_Variance': min(variance_history) if len(variance_history) > 0 else 0.0,
}

```

```

        'Gradient_Indicator': 0.0,
        'Mean_Gradient': 0.0,
        'Std_Gradient': 0.0,
        'Barren_Plateau_Status': 'N/A',
        # Store histories
        '_convergence_history': convergence_history,
        '_variance_history': variance_history,
        '_fidelity_history': [],
        '_gradient_history': []
    }

print(" Benchmark framework defined w/ debugging")

```

Benchmark framework defined w/ debugging

1.5 Step 5: Define Individual Ansätze (4 Different Implementations)

```
[15]: # Get problem parameters
num_qubits = problem.num_spatial_orbitals * 2
num_spatial_orbitals = problem.num_spatial_orbitals
num_particles = problem.num_particles

print(f"System parameters:")
print(f"  Number of qubits: {num_qubits}")
print(f"  Spatial orbitals: {num_spatial_orbitals}")
print(f"  Particles: {num_particles}")
print(f"\n{'='*70}")

# Create Hartree-Fock initial state (used by all ansätze)
hf_state = HartreeFock(
    num_spatial_orbitals,
    num_particles,
    mapper,
)

print("\n  Hartree-Fock initial state created")
print(f"  HF state qubits: {hf_state.num_qubits}")
print(f"\n{'='*70}\n")
```

System parameters:

```

Number of qubits: 8
Spatial orbitals: 4
Particles: (1, 1)
=====
```

```
Hartree-Fock initial state created
HF state qubits: 8
```

```

=====
[16]: from qiskit.circuit.library import TwoLocal
# =====
# ANSATZ 1: UCCSD (Unitary Coupled Cluster Singles and Doubles)
# =====
print("Creating Ansatz 1: UCCSD")
print("-" * 70)

ansatz_1_UCCSD = UCCSD(
    num_spatial_orbitals,
    num_particles,
    mapper,
    initial_state=hf_state,
)

print(f" UCCSD ansatz created")
print(f" Parameters: {ansatz_1_UCCSD.num_parameters}")
print(f" Qubits: {ansatz_1_UCCSD.num_qubits}")

# =====
# ANSATZ 2: UpCCGSD
# =====
print(f"\n{'='*70}")
print("Creating Ansatz 2: UpCCGSD: k = 2")
print("-" * 70)

def generate_upccgsd_excitations(num_spatial_orbitals, num_particles):
    """
    Generates the precise list of excitations for the UpCCGSD ansatz.
    """
    excitations = []

    # Loop over all unique pairs of spatial orbitals (p, q)
    for p in range(num_spatial_orbitals):
        for q in range(p + 1, num_spatial_orbitals):

            # 1. Generalized Singles (Spin-conserving): p -> q
            # Alpha: (2p,) -> (2q,)
            excitations.append((2 * p,), (2 * q,)))
            # Beta: (2p+1,) -> (2q+1,)
            excitations.append(((2 * p + 1,), (2 * q + 1,)))

    # 2. Generalized Pair Doubles (Zero-seniority)
    # Annihilate pair in p (2p, 2p+1), Create pair in q (2q, 2q+1)

```

```

        excitations.append(((2 * p, 2 * p + 1), (2 * q, 2 * q + 1)))

    return excitations

# Create the Exact UpCCGSD Ansatz manually
k_layers = 2

ansatz_2_UpCCGSD = UCC(
    num_spatial_orbitals=problem.num_spatial_orbitals,
    num_particles=problem.num_particles,
    qubit_mapper=mapper,
    initial_state=HartreeFock(
        problem.num_spatial_orbitals,
        problem.num_particles,
        mapper,
    ),
    # CORRECTED: Pass the function object, DO NOT call it ()
    excitations=generate_upccgsd_excitations,
    reps=k_layers
)

print(f" UpCCGSD ansatz created")
print(f" Parameters: {ansatz_2_UpCCGSD.num_parameters}")
print(f" Qubits: {ansatz_2_UpCCGSD.num_qubits}")
print(f" Reps: 3, Entanglement: linear")

# =====
# ANSATZ 3: TwoLocal (RY-RZ rotations with CX entanglement)
# =====
# print(f"\n{'='*70})
# =====
# ANSATZ 3: PC-HEA (Particle-Conserving Hardware-Efficient Ansatz)
# =====
print(f"\n{'='*70}")
print("Creating Ansatz 3: PC-HEA")
print("-" * 70)

# Create particle-conserving hardware-efficient ansatz (PC-HEA)
ansatz_3_PC_HEA = ExcitationPreserving(
    num_qubits=qubit_op.num_qubits,
    mode="fsim",           # particle-conserving entangling gate
    entanglement="linear", # linear entanglement
    reps=4,                # depth; increase if you want more expressivity
    initial_state=HartreeFock(
        problem.num_spatial_orbitals,
        problem.num_particles,
        mapper,
)

```

```

    )
)

# Prepend Hartree-Fock initial state
# HF state already set via initial_state parameter - no need to compose again

print(f" PC-HEA ansatz created")
print(f" Parameters: {ansatz_3_PC_HEA.num_parameters}")
print(f" Qubits: {ansatz_3_PC_HEA.num_qubits}")
print(f" Mode: fsim (Particle Conserving)")
print(f" Entanglement: linear, Reps: 4")

print(f"\n{'='*70}\n")

# ANSATZ 4: QEB (Qubit Excitation-Based)
# =====
print(f"\n{'='*70}")
print("Creating Ansatz 4: QEB (Qubit Excitation-Based)")
print("-" * 70)

from qeb_ansatz import QEBAbsatz

ansatz_4_QEB_8q = QEBAbsatz(
    num_qubits=num_qubits,
    num_particles=num_particles,
    num_spatial_orbitals=num_spatial_orbitals,
    depth=1,
    include_double=True,
    use_hartree_fock_init=True,
    mapper=mapper,
)
print(f" QEB_8q ansatz created")
print(f" Parameters: {ansatz_4_QEB_8q.num_parameters}")
print(f" Qubits: {ansatz_4_QEB_8q.num_qubits}")
print(f" Depth: 1")
print(f" Single excitations: {len(ansatz_4_QEB_8q.single_excitations)}")
print(f" Double excitations: {len(ansatz_4_QEB_8q.double_excitations)}")

print(f"\n{'='*70}\n")
print(" 4 ansätze created (all using 8-qubit Hamiltonian)")

```

Creating Ansatz 1: UCCSD

```

UCCSD ansatz created
Parameters: 15
Qubits: 8

```

```

=====
Creating Ansatz 2: UpCCGSD: k = 2
-----
UpCCGSD ansatz created
Parameters: 36
Qubits: 8
Reps: 3, Entanglement: linear

=====
Creating Ansatz 3: PC-HEA
-----
PC-HEA ansatz created
Parameters: 96
Qubits: 8
Mode: fsim (Particle Conserving)
Entanglement: linear, Reps: 4

=====
Creating Ansatz 4: QEB (Qubit Excitation-Based)
-----
QEB_8q ansatz created
Parameters: 50
Qubits: 8
Depth: 1
Single excitations: 12
Double excitations: 38

=====
4 ansätze created (all using 8-qubit Hamiltonian)

/var/folders/vv/d2w1vm213_b1g_0lt8qbw49r0000gn/T/ipykernel_20154/449189320.py:82
: DeprecationWarning: The class
``qiskit.circuit.library.n_local.excitation_preserving.ExcitationPreserving`` is
deprecated as of Qiskit 2.1. It will be removed in Qiskit 3.0. Use the function
qiskit.circuit.library.excitation_preserving instead.
    ansatz_3_PC_HEA = ExcitationPreserving(

```

[17]: # ======
Create dictionary of all ansätze (ONLY 3 ANSÄTZE)
======
ansatz_dict = {
 'UCCSD': ansatz_1_UCCSD,
 'UpCCGSD': ansatz_2_UpCCGSD,

```

'PC-HEA': ansatz_3_PC_HEA,
'QEB-8q': ansatz_4_QEB_8q,
'QEB-4q': None
}

# Configuration: Number of runs per ansatz
NUM_RUNS = 3

# Display summary
print("=*70)
print("ANSATZ DICTIONARY CREATED (3 ANSÄTZE)")
print("=*70)
print(f"\nTotal ansätze defined: {len(ansatz_dict)}")
print(f"Runs per ansatz: {NUM_RUNS}")
print(f"Total benchmarks: {len(ansatz_dict) * NUM_RUNS}")
print("\n" + "-*70)
print("Ansatz Summary:")
print("-*70)

for name, ansatz in ansatz_dict.items():
    if ansatz is None:
        print(f" {name:20s} | Special pipeline (see QEB benchmark cell)")
    else:
        print(f" {name:20s} | Params: {ansatz.num_parameters:3d} | Qubits:{ansatz.num_qubits}")

print("=*70)
print("\n Ready to run benchmarks with 3 ansätze!\n")

```

=====
ANSATZ DICTIONARY CREATED (3 ANSÄTZE)
=====

Total ansätze defined: 5

Runs per ansatz: 3

Total benchmarks: 15

Ansatz Summary:

UCCSD	Params: 15 Qubits: 8
UpCCGSD	Params: 36 Qubits: 8
PC-HEA	Params: 96 Qubits: 8
QEB-8q	Params: 50 Qubits: 8
QEB-4q	Special pipeline (see QEB benchmark cell)

=====
Ready to run benchmarks with 3 ansätze!

```
[18]: # =====
# QUICK TEST: Run just PC-HEA Run 1
# =====

print("=="*80)
print("QUICK TEST: Running PC-HEA only")
print("=="*80)

result = run_vqe_benchmark(
    ansatz=ansatz_3_PC_HEA,  # ← PC-HEA ansatz
    ansatz_name='PC-HEA',
    run_number=1,
    qubit_op=qubit_op,
    exact_electronic=exact_electronic,
    exact_state=exact_state,
    problem=problem,
    maxiter=300
)

print("\n" + "=="*80)
print("TEST COMPLETE")
print("=="*80)
```

=====

QUICK TEST: Running PC-HEA only

=====

=====

Running: PC-HEA - Run #1
Optimizer: COBYLA (maxiter=300)
Parameters: 96, Depth: 32

=====

Starting VQE optimization now...

Eval 1: E=-1.058862 Ha, Error=2.006 mHa
Eval 2: E=-1.058862 Ha, Error=2.006 mHa
Eval 3: E=-1.058862 Ha, Error=2.006 mHa
Eval 4: E=-1.058862 Ha, Error=2.006 mHa
Eval 5: E=-1.058862 Ha, Error=2.006 mHa
Eval 6: E=-1.058862 Ha, Error=2.006 mHa
Eval 7: E=-1.058862 Ha, Error=2.006 mHa
Eval 8: E=-1.058862 Ha, Error=2.006 mHa
Eval 9: E=-1.058862 Ha, Error=2.006 mHa
Eval 10: E=-0.951842 Ha, Error=109.026 mHa
Eval 11: E=-1.058862 Ha, Error=2.006 mHa
Eval 12: E=-1.058811 Ha, Error=2.057 mHa
Eval 13: E=-1.058862 Ha, Error=2.006 mHa

Eval 14: E=-1.058862 Ha, Error=2.006 mHa
Eval 15: E=-1.058862 Ha, Error=2.006 mHa
Eval 16: E=-0.935407 Ha, Error=125.461 mHa
Eval 17: E=-1.058862 Ha, Error=2.006 mHa
Eval 18: E=-0.947128 Ha, Error=113.740 mHa
Eval 19: E=-1.058862 Ha, Error=2.006 mHa
Eval 20: E=-1.058863 Ha, Error=2.005 mHa
Eval 21: E=-1.058863 Ha, Error=2.005 mHa
Eval 22: E=-1.058863 Ha, Error=2.005 mHa
Eval 23: E=-1.058863 Ha, Error=2.005 mHa
Eval 24: E=-1.058817 Ha, Error=2.051 mHa
Eval 25: E=-1.058819 Ha, Error=2.049 mHa
Eval 26: E=-1.058863 Ha, Error=2.005 mHa
Eval 27: E=-1.058842 Ha, Error=2.026 mHa
Eval 28: E=-1.058849 Ha, Error=2.019 mHa
Eval 29: E=-1.058872 Ha, Error=1.996 mHa
Eval 30: E=-1.058871 Ha, Error=1.997 mHa
Eval 31: E=-1.058872 Ha, Error=1.996 mHa
Eval 32: E=-0.951283 Ha, Error=109.585 mHa
Eval 33: E=-1.058872 Ha, Error=1.996 mHa
Eval 34: E=-1.058876 Ha, Error=1.992 mHa
Eval 35: E=-1.058876 Ha, Error=1.992 mHa
Eval 36: E=-1.058855 Ha, Error=2.013 mHa
Eval 37: E=-1.058876 Ha, Error=1.992 mHa
Eval 38: E=-0.935405 Ha, Error=125.464 mHa
Eval 39: E=-1.058876 Ha, Error=1.992 mHa
Eval 40: E=-0.948896 Ha, Error=111.972 mHa
Eval 41: E=-1.058876 Ha, Error=1.992 mHa
Eval 42: E=-1.058929 Ha, Error=1.939 mHa
Eval 43: E=-1.058929 Ha, Error=1.939 mHa
Eval 44: E=-1.058929 Ha, Error=1.939 mHa
Eval 45: E=-1.058929 Ha, Error=1.939 mHa
Eval 46: E=-1.058929 Ha, Error=1.939 mHa
Eval 47: E=-1.058929 Ha, Error=1.939 mHa
Eval 48: E=-1.058930 Ha, Error=1.938 mHa
Eval 49: E=-1.058942 Ha, Error=1.926 mHa
Eval 50: E=-1.058892 Ha, Error=1.976 mHa
Eval 51: E=-1.058932 Ha, Error=1.937 mHa
Eval 52: E=-1.058941 Ha, Error=1.927 mHa
Eval 53: E=-1.058942 Ha, Error=1.926 mHa
Eval 54: E=-0.951682 Ha, Error=109.186 mHa
Eval 55: E=-1.058942 Ha, Error=1.926 mHa
Eval 56: E=-1.058944 Ha, Error=1.924 mHa
Eval 57: E=-1.058944 Ha, Error=1.924 mHa
Eval 58: E=-1.058947 Ha, Error=1.921 mHa
Eval 59: E=-1.058947 Ha, Error=1.921 mHa
Eval 60: E=-0.933572 Ha, Error=127.296 mHa
Eval 61: E=-1.058947 Ha, Error=1.921 mHa

Eval 62: E=-0.950762 Ha, Error=110.106 mHa
Eval 63: E=-1.058947 Ha, Error=1.921 mHa
Eval 64: E=-1.058937 Ha, Error=1.931 mHa
Eval 65: E=-1.058947 Ha, Error=1.921 mHa
Eval 66: E=-1.058945 Ha, Error=1.923 mHa
Eval 67: E=-1.058947 Ha, Error=1.921 mHa
Eval 68: E=-1.058944 Ha, Error=1.924 mHa
Eval 69: E=-1.058948 Ha, Error=1.920 mHa
Eval 70: E=-1.058946 Ha, Error=1.922 mHa
Eval 71: E=-1.058942 Ha, Error=1.926 mHa
Eval 72: E=-1.058915 Ha, Error=1.953 mHa
Eval 73: E=-1.058934 Ha, Error=1.934 mHa
Eval 74: E=-1.058943 Ha, Error=1.925 mHa
Eval 75: E=-1.058948 Ha, Error=1.920 mHa
Eval 76: E=-0.950562 Ha, Error=110.306 mHa
Eval 77: E=-1.058948 Ha, Error=1.920 mHa
Eval 78: E=-1.058952 Ha, Error=1.916 mHa
Eval 79: E=-1.058952 Ha, Error=1.916 mHa
Eval 80: E=-1.058940 Ha, Error=1.928 mHa
Eval 81: E=-1.058952 Ha, Error=1.916 mHa
Eval 82: E=-0.933725 Ha, Error=127.143 mHa
Eval 83: E=-1.058952 Ha, Error=1.916 mHa
Eval 84: E=-0.951009 Ha, Error=109.859 mHa
Eval 85: E=-1.058952 Ha, Error=1.916 mHa
Eval 86: E=-1.058950 Ha, Error=1.918 mHa
Eval 87: E=-1.058952 Ha, Error=1.916 mHa
Eval 88: E=-1.058950 Ha, Error=1.918 mHa
Eval 89: E=-1.058952 Ha, Error=1.916 mHa
Eval 90: E=-1.058952 Ha, Error=1.916 mHa
Eval 91: E=-1.058952 Ha, Error=1.916 mHa
Eval 92: E=-1.058952 Ha, Error=1.916 mHa
Eval 93: E=-1.058952 Ha, Error=1.916 mHa
Eval 94: E=-1.058954 Ha, Error=1.914 mHa
Eval 95: E=-1.058954 Ha, Error=1.914 mHa
Eval 96: E=-1.058952 Ha, Error=1.916 mHa
Eval 97: E=-1.058954 Ha, Error=1.914 mHa
Eval 98: E=-0.800841 Ha, Error=260.027 mHa
Eval 99: E=-1.058954 Ha, Error=1.914 mHa
Eval 100: E=-1.027627 Ha, Error=33.241 mHa
Eval 101: E=-1.058954 Ha, Error=1.914 mHa
Eval 102: E=-1.031819 Ha, Error=29.049 mHa
Eval 103: E=-1.058954 Ha, Error=1.914 mHa
Eval 104: E=-1.018279 Ha, Error=42.589 mHa
Eval 105: E=-1.058954 Ha, Error=1.914 mHa
Eval 106: E=-0.953066 Ha, Error=107.803 mHa
Eval 107: E=-1.058954 Ha, Error=1.914 mHa
Eval 108: E=-0.914947 Ha, Error=145.921 mHa
Eval 109: E=-1.058954 Ha, Error=1.914 mHa

Eval 110: E=-0.924014 Ha, Error=136.854 mHa
Eval 111: E=-1.058953 Ha, Error=1.915 mHa
Eval 112: E=-1.020187 Ha, Error=40.682 mHa
Eval 113: E=-1.058953 Ha, Error=1.915 mHa
Eval 114: E=-0.957165 Ha, Error=103.703 mHa
Eval 115: E=-1.058953 Ha, Error=1.916 mHa
Eval 116: E=-0.941261 Ha, Error=119.607 mHa
Eval 117: E=-1.058957 Ha, Error=1.911 mHa
Eval 118: E=-0.949661 Ha, Error=111.207 mHa
Eval 119: E=-1.058959 Ha, Error=1.909 mHa
Eval 120: E=-0.920481 Ha, Error=140.387 mHa
Eval 121: E=-1.058964 Ha, Error=1.904 mHa
Eval 122: E=-1.040700 Ha, Error=20.168 mHa
Eval 123: E=-1.058966 Ha, Error=1.902 mHa
Eval 124: E=-0.920911 Ha, Error=139.957 mHa
Eval 125: E=-1.058966 Ha, Error=1.902 mHa
Eval 126: E=-0.955837 Ha, Error=105.032 mHa
Eval 127: E=-1.058957 Ha, Error=1.911 mHa
Eval 128: E=-0.970006 Ha, Error=90.862 mHa
Eval 129: E=-1.058966 Ha, Error=1.902 mHa
Eval 130: E=-1.041403 Ha, Error=19.465 mHa
Eval 131: E=-1.058954 Ha, Error=1.914 mHa
Eval 132: E=-0.944437 Ha, Error=116.431 mHa
Eval 133: E=-1.058966 Ha, Error=1.902 mHa
Eval 134: E=-0.949799 Ha, Error=111.069 mHa
Eval 135: E=-1.058974 Ha, Error=1.894 mHa
Eval 136: E=-0.786052 Ha, Error=274.816 mHa
Eval 137: E=-1.058971 Ha, Error=1.897 mHa
Eval 138: E=-1.034310 Ha, Error=26.558 mHa
Eval 139: E=-1.058969 Ha, Error=1.899 mHa
Eval 140: E=-0.920496 Ha, Error=140.372 mHa
Eval 141: E=-1.058972 Ha, Error=1.896 mHa
Eval 142: E=-0.938207 Ha, Error=122.661 mHa
Eval 143: E=-1.058957 Ha, Error=1.911 mHa
Eval 144: E=-0.927644 Ha, Error=133.224 mHa
Eval 145: E=-1.058974 Ha, Error=1.894 mHa
Eval 146: E=-0.937895 Ha, Error=122.974 mHa
Eval 147: E=-1.058967 Ha, Error=1.901 mHa
Eval 148: E=-0.953831 Ha, Error=107.038 mHa
Eval 149: E=-1.058973 Ha, Error=1.896 mHa
Eval 150: E=-0.952143 Ha, Error=108.725 mHa
Eval 151: E=-1.058971 Ha, Error=1.897 mHa
Eval 152: E=-0.957367 Ha, Error=103.502 mHa
Eval 153: E=-1.058974 Ha, Error=1.894 mHa
Eval 154: E=-0.788158 Ha, Error=272.710 mHa
Eval 155: E=-1.058972 Ha, Error=1.896 mHa
Eval 156: E=-1.043292 Ha, Error=17.576 mHa
Eval 157: E=-1.058974 Ha, Error=1.894 mHa

Eval 158: E=-0.926699 Ha, Error=134.169 mHa
Eval 159: E=-1.058974 Ha, Error=1.894 mHa
Eval 160: E=-0.791622 Ha, Error=269.246 mHa
Eval 161: E=-1.058971 Ha, Error=1.897 mHa
Eval 162: E=-1.047978 Ha, Error=12.890 mHa
Eval 163: E=-1.058974 Ha, Error=1.894 mHa
Eval 164: E=-0.794955 Ha, Error=265.914 mHa
Eval 165: E=-1.058974 Ha, Error=1.894 mHa
Eval 166: E=-0.949381 Ha, Error=111.488 mHa
Eval 167: E=-1.058974 Ha, Error=1.894 mHa
Eval 168: E=-0.796189 Ha, Error=264.679 mHa
Eval 169: E=-1.058975 Ha, Error=1.893 mHa
Eval 170: E=-0.923010 Ha, Error=137.858 mHa
Eval 171: E=-1.058970 Ha, Error=1.898 mHa
Eval 172: E=-1.056512 Ha, Error=4.356 mHa
Eval 173: E=-1.058974 Ha, Error=1.894 mHa
Eval 174: E=-0.834078 Ha, Error=226.790 mHa
Eval 175: E=-1.058982 Ha, Error=1.886 mHa
Eval 176: E=-0.923811 Ha, Error=137.057 mHa
Eval 177: E=-1.058975 Ha, Error=1.894 mHa
Eval 178: E=-1.035528 Ha, Error=25.340 mHa
Eval 179: E=-1.058976 Ha, Error=1.892 mHa
Eval 180: E=-0.858912 Ha, Error=201.956 mHa
Eval 181: E=-1.058982 Ha, Error=1.887 mHa
Eval 182: E=-0.955565 Ha, Error=105.303 mHa
Eval 183: E=-1.058982 Ha, Error=1.886 mHa
Eval 184: E=-0.954800 Ha, Error=106.068 mHa
Eval 185: E=-1.058982 Ha, Error=1.886 mHa
Eval 186: E=-1.045416 Ha, Error=15.452 mHa
Eval 187: E=-1.058981 Ha, Error=1.887 mHa
Eval 188: E=-0.931480 Ha, Error=129.389 mHa
Eval 189: E=-1.058982 Ha, Error=1.886 mHa
Eval 190: E=-0.941063 Ha, Error=119.805 mHa
Eval 191: E=-1.058982 Ha, Error=1.886 mHa
Eval 192: E=-0.924844 Ha, Error=136.025 mHa
Eval 193: E=-1.058982 Ha, Error=1.886 mHa
Eval 194: E=-1.051889 Ha, Error=8.979 mHa
Eval 195: E=-1.058982 Ha, Error=1.886 mHa
Eval 196: E=-0.843386 Ha, Error=217.482 mHa
Eval 197: E=-1.058958 Ha, Error=1.910 mHa
Eval 198: E=-0.944533 Ha, Error=116.336 mHa
Eval 199: E=-1.058982 Ha, Error=1.886 mHa
Eval 200: E=-0.962078 Ha, Error=98.790 mHa
Eval 201: E=-1.058982 Ha, Error=1.887 mHa
Eval 202: E=-0.961460 Ha, Error=99.409 mHa
Eval 203: E=-1.058982 Ha, Error=1.886 mHa
Eval 204: E=-0.970885 Ha, Error=89.983 mHa
Eval 205: E=-1.058982 Ha, Error=1.887 mHa

Eval 206: E=-0.917746 Ha, Error=143.122 mHa
Eval 207: E=-1.058982 Ha, Error=1.887 mHa
Eval 208: E=-0.947421 Ha, Error=113.447 mHa
Eval 209: E=-1.058982 Ha, Error=1.886 mHa
Eval 210: E=-0.922899 Ha, Error=137.969 mHa
Eval 211: E=-1.058982 Ha, Error=1.886 mHa
Eval 212: E=-1.040531 Ha, Error=20.337 mHa
Eval 213: E=-1.058969 Ha, Error=1.899 mHa
Eval 214: E=-0.954095 Ha, Error=106.773 mHa
Eval 215: E=-1.058976 Ha, Error=1.892 mHa
Eval 216: E=-1.017374 Ha, Error=43.494 mHa
Eval 217: E=-1.058982 Ha, Error=1.886 mHa
Eval 218: E=-0.936812 Ha, Error=124.056 mHa
Eval 219: E=-1.058982 Ha, Error=1.886 mHa
Eval 220: E=-1.017188 Ha, Error=43.680 mHa
Eval 221: E=-1.058982 Ha, Error=1.886 mHa
Eval 222: E=-0.846387 Ha, Error=214.481 mHa
Eval 223: E=-1.058983 Ha, Error=1.885 mHa
Eval 224: E=-0.942248 Ha, Error=118.620 mHa
Eval 225: E=-1.058983 Ha, Error=1.885 mHa
Eval 226: E=-1.054580 Ha, Error=6.288 mHa
Eval 227: E=-1.058983 Ha, Error=1.885 mHa
Eval 228: E=-0.851103 Ha, Error=209.765 mHa
Eval 229: E=-1.058983 Ha, Error=1.886 mHa
Eval 230: E=-0.927957 Ha, Error=132.911 mHa
Eval 231: E=-1.058983 Ha, Error=1.886 mHa
Eval 232: E=-0.957137 Ha, Error=103.731 mHa
Eval 233: E=-1.058982 Ha, Error=1.886 mHa
Eval 234: E=-0.850766 Ha, Error=210.102 mHa
Eval 235: E=-1.058982 Ha, Error=1.887 mHa
Eval 236: E=-1.026634 Ha, Error=34.234 mHa
Eval 237: E=-1.058983 Ha, Error=1.885 mHa
Eval 238: E=-0.850785 Ha, Error=210.083 mHa
Eval 239: E=-1.058983 Ha, Error=1.885 mHa
Eval 240: E=-0.918530 Ha, Error=142.338 mHa
Eval 241: E=-1.058983 Ha, Error=1.885 mHa
Eval 242: E=-0.854823 Ha, Error=206.045 mHa
Eval 243: E=-1.058983 Ha, Error=1.885 mHa
Eval 244: E=-1.050471 Ha, Error=10.397 mHa
Eval 245: E=-1.058984 Ha, Error=1.884 mHa
Eval 246: E=-1.041180 Ha, Error=19.688 mHa
Eval 247: E=-1.058984 Ha, Error=1.884 mHa
Eval 248: E=-0.918354 Ha, Error=142.515 mHa
Eval 249: E=-1.058983 Ha, Error=1.885 mHa
Eval 250: E=-0.868507 Ha, Error=192.361 mHa
Eval 251: E=-1.058984 Ha, Error=1.884 mHa
Eval 252: E=-0.932533 Ha, Error=128.335 mHa
Eval 253: E=-1.058983 Ha, Error=1.885 mHa

```
Eval 254: E=-1.044022 Ha, Error=16.846 mHa
Eval 255: E=-1.058984 Ha, Error=1.884 mHa
Eval 256: E=-0.942309 Ha, Error=118.559 mHa
Eval 257: E=-1.049398 Ha, Error=11.470 mHa
Eval 258: E=-0.910565 Ha, Error=150.303 mHa
Eval 259: E=-1.051369 Ha, Error=9.499 mHa
Eval 260: E=-0.936177 Ha, Error=124.691 mHa
Eval 261: E=-1.058985 Ha, Error=1.884 mHa
Eval 262: E=-0.948799 Ha, Error=112.069 mHa
Eval 263: E=-1.058985 Ha, Error=1.884 mHa
Eval 264: E=-1.003913 Ha, Error=56.955 mHa
Eval 265: E=-1.058984 Ha, Error=1.884 mHa
Eval 266: E=-0.957475 Ha, Error=103.393 mHa
Eval 267: E=-1.058984 Ha, Error=1.885 mHa
Eval 268: E=-0.942536 Ha, Error=118.332 mHa
Eval 269: E=-1.058984 Ha, Error=1.884 mHa
Eval 270: E=-0.969020 Ha, Error=91.849 mHa
Eval 271: E=-1.058983 Ha, Error=1.885 mHa
Eval 272: E=-0.968652 Ha, Error=92.217 mHa
Eval 273: E=-1.058983 Ha, Error=1.885 mHa
Eval 274: E=-0.877364 Ha, Error=183.504 mHa
Eval 275: E=-1.058982 Ha, Error=1.886 mHa
Eval 276: E=-0.959603 Ha, Error=101.265 mHa
Eval 277: E=-1.058978 Ha, Error=1.890 mHa
Eval 278: E=-0.973265 Ha, Error=87.603 mHa
Eval 279: E=-1.058983 Ha, Error=1.885 mHa
Eval 280: E=-0.923851 Ha, Error=137.017 mHa
Eval 281: E=-1.052053 Ha, Error=8.815 mHa
Eval 282: E=-0.882832 Ha, Error=178.036 mHa
Eval 283: E=-1.058982 Ha, Error=1.886 mHa
Eval 284: E=-0.906786 Ha, Error=154.082 mHa
Eval 285: E=-1.048926 Ha, Error=11.942 mHa
Eval 286: E=-0.894783 Ha, Error=166.085 mHa
Eval 287: E=-1.058982 Ha, Error=1.886 mHa
Eval 288: E=-0.948976 Ha, Error=111.892 mHa
Eval 289: E=-1.052518 Ha, Error=8.350 mHa
Eval 290: E=-0.901333 Ha, Error=159.535 mHa
Eval 291: E=-1.058976 Ha, Error=1.892 mHa
Eval 292: E=-0.942956 Ha, Error=117.912 mHa
Eval 293: E=-1.058983 Ha, Error=1.885 mHa
Eval 294: E=-0.900703 Ha, Error=160.165 mHa
Eval 295: E=-1.058984 Ha, Error=1.885 mHa
Eval 296: E=-0.948908 Ha, Error=111.960 mHa
Eval 297: E=-1.058982 Ha, Error=1.886 mHa
Eval 298: E=-0.900857 Ha, Error=160.011 mHa
Eval 299: E=-1.058973 Ha, Error=1.895 mHa
Eval 300: E=-0.907131 Ha, Error=153.737 mHa
VQE compute_minimum_eigenvalue took: 1.7s
```

```
Completed in 1.7s
  Function evaluations: 300
  Callback captured: 300 points
  Energy Error: 1.883621e-03 Ha (0.1776%)
  Fidelity: 0.996781
  Convergence: 300/300 iterations
```

```
=====
TEST COMPLETE
=====
```

```
[19]: print("=*80)
print("TESTING UCCSD")
print("=*80)

result = run_vqe_benchmark(
    ansatz=ansatz_1_UCCSD,  # ← UCCSD this time
    ansatz_name='UCCSD',
    run_number=1,
    qubit_op=qubit_op,
    exact_electronic=exact_electronic,
    exact_state=exact_state,
    problem=problem,
    maxiter=300
)

=====
TESTING UCCSD
=====

=====
Running: UCCSD - Run #1
Optimizer: COBYLA (maxiter=300)
Parameters: 15, Depth: 16
=====
Starting VQE optimization now...
/Users/eric_jin/.pyenv/versions/3.11.9/lib/python3.11/site-
packages/scipy/sparse/linalg/_dsolve/linsolve.py:606: SparseEfficiencyWarning:
splu converted its input to CSC format
    return splu(A).solve
/Users/eric_jin/.pyenv/versions/3.11.9/lib/python3.11/site-
packages/scipy/sparse/linalg/_matfuncs.py:707: SparseEfficiencyWarning: spsolve
is more efficient when sparse b is in the CSC matrix format
    return spsolve(Q, P)

    Eval 1: E=-1.058211 Ha, Error=2.657 mHa
    Eval 2: E=-0.949848 Ha, Error=111.021 mHa
```

Eval 3: E=-0.916322 Ha, Error=144.546 mHa
Eval 4: E=-0.915135 Ha, Error=145.733 mHa
Eval 5: E=-0.951391 Ha, Error=109.477 mHa
Eval 6: E=-0.915127 Ha, Error=145.741 mHa
Eval 7: E=-0.916747 Ha, Error=144.121 mHa
Eval 8: E=-0.559076 Ha, Error=501.792 mHa
Eval 9: E=-0.601074 Ha, Error=459.794 mHa
Eval 10: E=-0.604744 Ha, Error=456.124 mHa
Eval 11: E=-0.612346 Ha, Error=448.522 mHa
Eval 12: E=-0.568154 Ha, Error=492.714 mHa
Eval 13: E=-0.609360 Ha, Error=451.508 mHa
Eval 14: E=-0.620164 Ha, Error=440.704 mHa
Eval 15: E=-0.616726 Ha, Error=444.142 mHa
Eval 16: E=-0.563561 Ha, Error=497.307 mHa
Eval 17: E=-0.701190 Ha, Error=359.678 mHa
Eval 18: E=-0.896241 Ha, Error=164.627 mHa
Eval 19: E=-1.031277 Ha, Error=29.591 mHa
Eval 20: E=-1.057176 Ha, Error=3.692 mHa
Eval 21: E=-1.047929 Ha, Error=12.939 mHa
Eval 22: E=-1.056876 Ha, Error=3.992 mHa
Eval 23: E=-1.048664 Ha, Error=12.204 mHa
Eval 24: E=-1.057217 Ha, Error=3.651 mHa
Eval 25: E=-1.050315 Ha, Error=10.553 mHa
Eval 26: E=-1.057499 Ha, Error=3.369 mHa
Eval 27: E=-1.050839 Ha, Error=10.030 mHa
Eval 28: E=-1.057560 Ha, Error=3.308 mHa
Eval 29: E=-1.051623 Ha, Error=9.245 mHa
Eval 30: E=-1.057525 Ha, Error=3.343 mHa
Eval 31: E=-1.052425 Ha, Error=8.443 mHa
Eval 32: E=-1.056327 Ha, Error=4.541 mHa
Eval 33: E=-1.055581 Ha, Error=5.287 mHa
Eval 34: E=-1.053980 Ha, Error=6.888 mHa
Eval 35: E=-1.057704 Ha, Error=3.164 mHa
Eval 36: E=-1.054783 Ha, Error=6.085 mHa
Eval 37: E=-1.058468 Ha, Error=2.400 mHa
Eval 38: E=-1.059532 Ha, Error=1.336 mHa
Eval 39: E=-1.058905 Ha, Error=1.963 mHa
Eval 40: E=-1.059477 Ha, Error=1.392 mHa
Eval 41: E=-1.059473 Ha, Error=1.395 mHa
Eval 42: E=-1.059485 Ha, Error=1.383 mHa
Eval 43: E=-1.059728 Ha, Error=1.140 mHa
Eval 44: E=-1.059614 Ha, Error=1.254 mHa
Eval 45: E=-1.059866 Ha, Error=1.002 mHa
Eval 46: E=-1.060255 Ha, Error=0.613 mHa
Eval 47: E=-1.060322 Ha, Error=0.546 mHa
Eval 48: E=-1.060385 Ha, Error=0.483 mHa
Eval 49: E=-1.060463 Ha, Error=0.405 mHa
Eval 50: E=-1.060356 Ha, Error=0.512 mHa

Eval 51: E=-1.060450 Ha, Error=0.418 mHa
Eval 52: E=-1.060562 Ha, Error=0.306 mHa
Eval 53: E=-1.060359 Ha, Error=0.510 mHa
Eval 54: E=-1.060546 Ha, Error=0.322 mHa
Eval 55: E=-1.060624 Ha, Error=0.244 mHa
Eval 56: E=-1.060598 Ha, Error=0.270 mHa
Eval 57: E=-1.060601 Ha, Error=0.267 mHa
Eval 58: E=-1.060660 Ha, Error=0.208 mHa
Eval 59: E=-1.060713 Ha, Error=0.155 mHa
Eval 60: E=-1.060691 Ha, Error=0.177 mHa
Eval 61: E=-1.060689 Ha, Error=0.179 mHa
Eval 62: E=-1.060687 Ha, Error=0.181 mHa
Eval 63: E=-1.060685 Ha, Error=0.184 mHa
Eval 64: E=-1.060706 Ha, Error=0.162 mHa
Eval 65: E=-1.060684 Ha, Error=0.184 mHa
Eval 66: E=-1.060652 Ha, Error=0.216 mHa
Eval 67: E=-1.060678 Ha, Error=0.190 mHa
Eval 68: E=-1.060662 Ha, Error=0.206 mHa
Eval 69: E=-1.060723 Ha, Error=0.145 mHa
Eval 70: E=-1.060659 Ha, Error=0.210 mHa
Eval 71: E=-1.060699 Ha, Error=0.169 mHa
Eval 72: E=-1.060690 Ha, Error=0.178 mHa
Eval 73: E=-1.060731 Ha, Error=0.137 mHa
Eval 74: E=-1.060731 Ha, Error=0.137 mHa
Eval 75: E=-1.060729 Ha, Error=0.139 mHa
Eval 76: E=-1.060739 Ha, Error=0.130 mHa
Eval 77: E=-1.060741 Ha, Error=0.127 mHa
Eval 78: E=-1.060746 Ha, Error=0.122 mHa
Eval 79: E=-1.060750 Ha, Error=0.119 mHa
Eval 80: E=-1.060751 Ha, Error=0.117 mHa
Eval 81: E=-1.060755 Ha, Error=0.113 mHa
Eval 82: E=-1.060758 Ha, Error=0.110 mHa
Eval 83: E=-1.060761 Ha, Error=0.107 mHa
Eval 84: E=-1.060762 Ha, Error=0.107 mHa
Eval 85: E=-1.060760 Ha, Error=0.108 mHa
Eval 86: E=-1.060758 Ha, Error=0.110 mHa
Eval 87: E=-1.060764 Ha, Error=0.104 mHa
Eval 88: E=-1.060764 Ha, Error=0.104 mHa
Eval 89: E=-1.060764 Ha, Error=0.104 mHa
Eval 90: E=-1.060763 Ha, Error=0.105 mHa
Eval 91: E=-1.060770 Ha, Error=0.098 mHa
Eval 92: E=-1.060770 Ha, Error=0.098 mHa
Eval 93: E=-1.060767 Ha, Error=0.101 mHa
Eval 94: E=-1.060779 Ha, Error=0.089 mHa
Eval 95: E=-1.060786 Ha, Error=0.083 mHa
Eval 96: E=-1.060792 Ha, Error=0.076 mHa
Eval 97: E=-1.060798 Ha, Error=0.070 mHa
Eval 98: E=-1.060802 Ha, Error=0.066 mHa

Eval 99: E=-1.060808 Ha, Error=0.060 mHa
Eval 100: E=-1.060810 Ha, Error=0.058 mHa
Eval 101: E=-1.060812 Ha, Error=0.057 mHa
Eval 102: E=-1.060814 Ha, Error=0.054 mHa
Eval 103: E=-1.060815 Ha, Error=0.053 mHa
Eval 104: E=-1.060815 Ha, Error=0.054 mHa
Eval 105: E=-1.060814 Ha, Error=0.054 mHa
Eval 106: E=-1.060817 Ha, Error=0.051 mHa
Eval 107: E=-1.060819 Ha, Error=0.049 mHa
Eval 108: E=-1.060819 Ha, Error=0.049 mHa
Eval 109: E=-1.060819 Ha, Error=0.049 mHa
Eval 110: E=-1.060818 Ha, Error=0.050 mHa
Eval 111: E=-1.060823 Ha, Error=0.045 mHa
Eval 112: E=-1.060828 Ha, Error=0.040 mHa
Eval 113: E=-1.060832 Ha, Error=0.036 mHa
Eval 114: E=-1.060833 Ha, Error=0.035 mHa
Eval 115: E=-1.060836 Ha, Error=0.032 mHa
Eval 116: E=-1.060840 Ha, Error=0.029 mHa
Eval 117: E=-1.060841 Ha, Error=0.027 mHa
Eval 118: E=-1.060841 Ha, Error=0.027 mHa
Eval 119: E=-1.060840 Ha, Error=0.028 mHa
Eval 120: E=-1.060844 Ha, Error=0.025 mHa
Eval 121: E=-1.060844 Ha, Error=0.024 mHa
Eval 122: E=-1.060846 Ha, Error=0.022 mHa
Eval 123: E=-1.060848 Ha, Error=0.020 mHa
Eval 124: E=-1.060849 Ha, Error=0.019 mHa
Eval 125: E=-1.060852 Ha, Error=0.017 mHa
Eval 126: E=-1.060852 Ha, Error=0.016 mHa
Eval 127: E=-1.060853 Ha, Error=0.015 mHa
Eval 128: E=-1.060852 Ha, Error=0.016 mHa
Eval 129: E=-1.060852 Ha, Error=0.016 mHa
Eval 130: E=-1.060854 Ha, Error=0.014 mHa
Eval 131: E=-1.060857 Ha, Error=0.012 mHa
Eval 132: E=-1.060858 Ha, Error=0.010 mHa
Eval 133: E=-1.060860 Ha, Error=0.009 mHa
Eval 134: E=-1.060861 Ha, Error=0.007 mHa
Eval 135: E=-1.060861 Ha, Error=0.007 mHa
Eval 136: E=-1.060860 Ha, Error=0.008 mHa
Eval 137: E=-1.060861 Ha, Error=0.007 mHa
Eval 138: E=-1.060862 Ha, Error=0.006 mHa
Eval 139: E=-1.060863 Ha, Error=0.005 mHa
Eval 140: E=-1.060863 Ha, Error=0.005 mHa
Eval 141: E=-1.060864 Ha, Error=0.004 mHa
Eval 142: E=-1.060864 Ha, Error=0.005 mHa
Eval 143: E=-1.060864 Ha, Error=0.004 mHa
Eval 144: E=-1.060864 Ha, Error=0.004 mHa
Eval 145: E=-1.060865 Ha, Error=0.003 mHa
Eval 146: E=-1.060865 Ha, Error=0.003 mHa

Eval 147: E=-1.060865 Ha, Error=0.003 mHa
Eval 148: E=-1.060866 Ha, Error=0.002 mHa
Eval 149: E=-1.060865 Ha, Error=0.003 mHa
Eval 150: E=-1.060866 Ha, Error=0.002 mHa
Eval 151: E=-1.060866 Ha, Error=0.002 mHa
Eval 152: E=-1.060866 Ha, Error=0.002 mHa
Eval 153: E=-1.060866 Ha, Error=0.002 mHa
Eval 154: E=-1.060866 Ha, Error=0.002 mHa
Eval 155: E=-1.060866 Ha, Error=0.002 mHa
Eval 156: E=-1.060866 Ha, Error=0.002 mHa
Eval 157: E=-1.060866 Ha, Error=0.002 mHa
Eval 158: E=-1.060866 Ha, Error=0.003 mHa
Eval 159: E=-1.060866 Ha, Error=0.002 mHa
Eval 160: E=-1.060866 Ha, Error=0.002 mHa
Eval 161: E=-1.060866 Ha, Error=0.002 mHa
Eval 162: E=-1.060866 Ha, Error=0.002 mHa
Eval 163: E=-1.060866 Ha, Error=0.002 mHa
Eval 164: E=-1.060867 Ha, Error=0.001 mHa
Eval 165: E=-1.060866 Ha, Error=0.002 mHa
Eval 166: E=-1.060867 Ha, Error=0.001 mHa
Eval 167: E=-1.060867 Ha, Error=0.001 mHa
Eval 168: E=-1.060867 Ha, Error=0.002 mHa
Eval 169: E=-1.060867 Ha, Error=0.001 mHa
Eval 170: E=-1.060867 Ha, Error=0.001 mHa
Eval 171: E=-1.060867 Ha, Error=0.001 mHa
Eval 172: E=-1.060867 Ha, Error=0.001 mHa
Eval 173: E=-1.060867 Ha, Error=0.001 mHa
Eval 174: E=-1.060867 Ha, Error=0.001 mHa
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Eval 176: E=-1.060867 Ha, Error=0.001 mHa
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Eval 179: E=-1.060867 Ha, Error=0.001 mHa
Eval 180: E=-1.060867 Ha, Error=0.001 mHa
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Eval 182: E=-1.060867 Ha, Error=0.001 mHa
Eval 183: E=-1.060867 Ha, Error=0.001 mHa
Eval 184: E=-1.060867 Ha, Error=0.001 mHa
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Eval 195: E=-1.060867 Ha, Error=0.001 mHa
Eval 196: E=-1.060867 Ha, Error=0.001 mHa
Eval 197: E=-1.060867 Ha, Error=0.001 mHa
Eval 198: E=-1.060868 Ha, Error=0.001 mHa
Eval 199: E=-1.060868 Ha, Error=0.001 mHa
Eval 200: E=-1.060868 Ha, Error=0.001 mHa
Eval 201: E=-1.060868 Ha, Error=0.001 mHa
Eval 202: E=-1.060868 Ha, Error=0.001 mHa
Eval 203: E=-1.060868 Ha, Error=0.000 mHa
Eval 204: E=-1.060868 Ha, Error=0.000 mHa
Eval 205: E=-1.060868 Ha, Error=0.000 mHa
Eval 206: E=-1.060868 Ha, Error=0.000 mHa
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Eval 210: E=-1.060868 Ha, Error=0.000 mHa
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Eval 229: E=-1.060868 Ha, Error=0.000 mHa
Eval 230: E=-1.060868 Ha, Error=0.000 mHa
Eval 231: E=-1.060868 Ha, Error=0.000 mHa
Eval 232: E=-1.060868 Ha, Error=0.000 mHa
Eval 233: E=-1.060868 Ha, Error=0.000 mHa
Eval 234: E=-1.060868 Ha, Error=0.000 mHa
Eval 235: E=-1.060868 Ha, Error=0.000 mHa
Eval 236: E=-1.060868 Ha, Error=0.000 mHa
Eval 237: E=-1.060868 Ha, Error=0.000 mHa
Eval 238: E=-1.060868 Ha, Error=0.000 mHa
Eval 239: E=-1.060868 Ha, Error=0.000 mHa
Eval 240: E=-1.060868 Ha, Error=0.000 mHa
Eval 241: E=-1.060868 Ha, Error=0.000 mHa
Eval 242: E=-1.060868 Ha, Error=0.000 mHa


```

Eval 291: E=-1.060868 Ha, Error=0.000 mHa
Eval 292: E=-1.060868 Ha, Error=0.000 mHa
Eval 293: E=-1.060868 Ha, Error=0.000 mHa
Eval 294: E=-1.060868 Ha, Error=0.000 mHa
Eval 295: E=-1.060868 Ha, Error=0.000 mHa
Eval 296: E=-1.060868 Ha, Error=0.000 mHa
Eval 297: E=-1.060868 Ha, Error=0.000 mHa
Eval 298: E=-1.060868 Ha, Error=0.000 mHa
Eval 299: E=-1.060868 Ha, Error=0.000 mHa
Eval 300: E=-1.060868 Ha, Error=0.000 mHa
VQE compute_minimum_eigenvalue took: 75.1s

```

```

Completed in 75.1s
Function evaluations: 300
Callback captured: 300 points
Energy Error: 2.768017e-09 Ha (0.0000%)
Fidelity: 1.000000
Convergence: 119/300 iterations

```

```
[20]: print("=="*80)
print("TESTING QEB-8q")
print("=="*80)

result = run_vqe_benchmark(
    ansatz=ansatz_4_QEB_8q,
    ansatz_name='QEB-8q',
    run_number=1,
    qubit_op=qubit_op,
    exact_electronic=exact_electronic,
    exact_state=exact_state,
    problem=problem,
    maxiter=300
)
```

```
=====
TESTING QEB-8q
=====

=====
Running: QEB-8q - Run #1
Optimizer: COBYLA (maxiter=300)
Parameters: 50, Depth: 149
=====

Starting VQE optimization now...
  Eval 1: E=-1.059016 Ha, Error=1.853 mHa
  Eval 2: E=-1.031874 Ha, Error=28.994 mHa
  Eval 3: E=-1.022609 Ha, Error=38.260 mHa
  Eval 4: E=-1.032442 Ha, Error=28.427 mHa
```

Eval 5: E=-1.031738 Ha, Error=29.130 mHa
Eval 6: E=-1.037294 Ha, Error=23.575 mHa
Eval 7: E=-1.032485 Ha, Error=28.383 mHa
Eval 8: E=-1.042575 Ha, Error=18.293 mHa
Eval 9: E=-1.047446 Ha, Error=13.422 mHa
Eval 10: E=-1.042366 Ha, Error=18.502 mHa
Eval 11: E=-1.043394 Ha, Error=17.474 mHa
Eval 12: E=-1.038061 Ha, Error=22.807 mHa
Eval 13: E=-1.043338 Ha, Error=17.530 mHa
Eval 14: E=-1.044835 Ha, Error=16.033 mHa
Eval 15: E=-1.050582 Ha, Error=10.287 mHa
Eval 16: E=-1.047507 Ha, Error=13.361 mHa
Eval 17: E=-1.048886 Ha, Error=11.982 mHa
Eval 18: E=-1.047607 Ha, Error=13.261 mHa
Eval 19: E=-1.048067 Ha, Error=12.801 mHa
Eval 20: E=-1.046781 Ha, Error=14.087 mHa
Eval 21: E=-1.048028 Ha, Error=12.840 mHa
Eval 22: E=-1.046606 Ha, Error=14.262 mHa
Eval 23: E=-1.047758 Ha, Error=13.110 mHa
Eval 24: E=-1.046460 Ha, Error=14.408 mHa
Eval 25: E=-1.046963 Ha, Error=13.905 mHa
Eval 26: E=-1.045614 Ha, Error=15.254 mHa
Eval 27: E=-1.046854 Ha, Error=14.014 mHa
Eval 27: E=-1.046854 Ha, Error=14.014 mHa
Eval 28: E=-1.047761 Ha, Error=13.107 mHa
Eval 29: E=-1.049133 Ha, Error=11.735 mHa
Eval 30: E=-1.047845 Ha, Error=13.023 mHa
Eval 31: E=-1.048345 Ha, Error=12.523 mHa
Eval 32: E=-1.047039 Ha, Error=13.829 mHa
Eval 33: E=-1.048281 Ha, Error=12.587 mHa
Eval 34: E=-1.048529 Ha, Error=12.339 mHa
Eval 35: E=-1.049725 Ha, Error=11.143 mHa
Eval 36: E=-1.048387 Ha, Error=12.481 mHa
Eval 37: E=-1.047961 Ha, Error=12.907 mHa
Eval 38: E=-1.046620 Ha, Error=14.248 mHa
Eval 39: E=-1.048027 Ha, Error=12.841 mHa
Eval 40: E=-1.049360 Ha, Error=11.509 mHa
Eval 41: E=-1.050697 Ha, Error=10.171 mHa
Eval 42: E=-1.049425 Ha, Error=11.444 mHa
Eval 43: E=-1.048923 Ha, Error=11.945 mHa
Eval 44: E=-1.047574 Ha, Error=13.294 mHa
Eval 45: E=-1.049024 Ha, Error=11.844 mHa
Eval 46: E=-1.047802 Ha, Error=13.067 mHa
Eval 47: E=-1.049193 Ha, Error=11.675 mHa
Eval 48: E=-1.047914 Ha, Error=12.954 mHa
Eval 49: E=-1.048399 Ha, Error=12.469 mHa
Eval 50: E=-1.047097 Ha, Error=13.772 mHa
Eval 51: E=-1.048355 Ha, Error=12.513 mHa

Eval 52: E=-0.914103 Ha, Error=146.765 mHa
Eval 53: E=-1.053068 Ha, Error=7.800 mHa
Eval 54: E=-1.049669 Ha, Error=11.200 mHa
Eval 55: E=-1.058962 Ha, Error=1.906 mHa
Eval 56: E=-1.058595 Ha, Error=2.273 mHa
Eval 57: E=-1.058949 Ha, Error=1.919 mHa
Eval 58: E=-1.058910 Ha, Error=1.958 mHa
Eval 59: E=-1.059012 Ha, Error=1.856 mHa
Eval 60: E=-1.058853 Ha, Error=2.015 mHa
Eval 61: E=-1.059024 Ha, Error=1.844 mHa
Eval 62: E=-1.058821 Ha, Error=2.048 mHa
Eval 63: E=-1.059026 Ha, Error=1.842 mHa
Eval 64: E=-1.057287 Ha, Error=3.582 mHa
Eval 65: E=-1.058977 Ha, Error=1.891 mHa
Eval 66: E=-1.058874 Ha, Error=1.995 mHa
Eval 67: E=-1.058989 Ha, Error=1.879 mHa
Eval 68: E=-1.059005 Ha, Error=1.863 mHa
Eval 69: E=-1.059001 Ha, Error=1.867 mHa
Eval 70: E=-1.058974 Ha, Error=1.894 mHa
Eval 71: E=-1.059018 Ha, Error=1.851 mHa
Eval 72: E=-1.058966 Ha, Error=1.902 mHa
Eval 73: E=-1.059019 Ha, Error=1.849 mHa
Eval 74: E=-1.058993 Ha, Error=1.875 mHa
Eval 75: E=-1.058989 Ha, Error=1.879 mHa
Eval 76: E=-1.058927 Ha, Error=1.941 mHa
Eval 77: E=-1.059024 Ha, Error=1.844 mHa
Eval 78: E=-1.058868 Ha, Error=2.000 mHa
Eval 79: E=-1.059006 Ha, Error=1.862 mHa
Eval 80: E=-1.058902 Ha, Error=1.967 mHa
Eval 81: E=-1.058998 Ha, Error=1.871 mHa
Eval 82: E=-1.058979 Ha, Error=1.889 mHa
Eval 83: E=-1.059009 Ha, Error=1.859 mHa
Eval 84: E=-1.058938 Ha, Error=1.930 mHa
Eval 85: E=-1.059001 Ha, Error=1.868 mHa
Eval 86: E=-1.058983 Ha, Error=1.886 mHa
Eval 87: E=-1.058987 Ha, Error=1.881 mHa
Eval 88: E=-1.058964 Ha, Error=1.904 mHa
Eval 89: E=-1.059010 Ha, Error=1.858 mHa
Eval 90: E=-1.058978 Ha, Error=1.890 mHa
Eval 91: E=-1.059037 Ha, Error=1.832 mHa
Eval 92: E=-1.058984 Ha, Error=1.884 mHa
Eval 93: E=-1.059020 Ha, Error=1.848 mHa
Eval 94: E=-1.058962 Ha, Error=1.906 mHa
Eval 95: E=-1.059023 Ha, Error=1.845 mHa
Eval 96: E=-1.058902 Ha, Error=1.966 mHa
Eval 97: E=-1.059033 Ha, Error=1.835 mHa
Eval 98: E=-1.058938 Ha, Error=1.930 mHa
Eval 99: E=-1.059044 Ha, Error=1.824 mHa

Eval 100: E=-1.058892 Ha, Error=1.976 mHa
Eval 101: E=-1.059042 Ha, Error=1.826 mHa
Eval 102: E=-1.058891 Ha, Error=1.977 mHa
Eval 103: E=-1.059046 Ha, Error=1.823 mHa
Eval 104: E=-1.058759 Ha, Error=2.109 mHa
Eval 105: E=-1.059016 Ha, Error=1.852 mHa
Eval 106: E=-1.058107 Ha, Error=2.761 mHa
Eval 107: E=-1.058728 Ha, Error=2.140 mHa
Eval 108: E=-1.059043 Ha, Error=1.826 mHa
Eval 109: E=-1.059041 Ha, Error=1.827 mHa
Eval 110: E=-1.059047 Ha, Error=1.821 mHa
Eval 111: E=-1.059043 Ha, Error=1.825 mHa
Eval 112: E=-1.059046 Ha, Error=1.822 mHa
Eval 113: E=-1.059043 Ha, Error=1.825 mHa
Eval 114: E=-1.059047 Ha, Error=1.821 mHa
Eval 115: E=-1.059043 Ha, Error=1.825 mHa
Eval 116: E=-1.059047 Ha, Error=1.821 mHa
Eval 117: E=-1.059044 Ha, Error=1.824 mHa
Eval 118: E=-1.059045 Ha, Error=1.823 mHa
Eval 119: E=-1.059047 Ha, Error=1.821 mHa
Eval 120: E=-1.059046 Ha, Error=1.822 mHa
Eval 121: E=-1.059038 Ha, Error=1.830 mHa
Eval 122: E=-1.059046 Ha, Error=1.822 mHa
Eval 123: E=-1.059046 Ha, Error=1.822 mHa
Eval 124: E=-1.059046 Ha, Error=1.822 mHa
Eval 125: E=-1.059048 Ha, Error=1.820 mHa
Eval 126: E=-1.059047 Ha, Error=1.822 mHa
Eval 127: E=-1.059048 Ha, Error=1.820 mHa
Eval 128: E=-1.059048 Ha, Error=1.820 mHa
Eval 129: E=-1.059049 Ha, Error=1.819 mHa
Eval 130: E=-1.059050 Ha, Error=1.818 mHa
Eval 131: E=-1.059049 Ha, Error=1.819 mHa
Eval 132: E=-1.059049 Ha, Error=1.819 mHa
Eval 133: E=-1.059048 Ha, Error=1.821 mHa
Eval 134: E=-1.059049 Ha, Error=1.819 mHa
Eval 135: E=-1.059049 Ha, Error=1.820 mHa
Eval 136: E=-1.059049 Ha, Error=1.819 mHa
Eval 137: E=-1.059047 Ha, Error=1.821 mHa
Eval 138: E=-1.059050 Ha, Error=1.818 mHa
Eval 139: E=-1.059049 Ha, Error=1.819 mHa
Eval 140: E=-1.059049 Ha, Error=1.819 mHa
Eval 141: E=-1.059048 Ha, Error=1.820 mHa
Eval 142: E=-1.059049 Ha, Error=1.819 mHa
Eval 143: E=-1.059049 Ha, Error=1.819 mHa
Eval 144: E=-1.059049 Ha, Error=1.819 mHa
Eval 145: E=-1.059050 Ha, Error=1.818 mHa
Eval 146: E=-1.059050 Ha, Error=1.818 mHa
Eval 147: E=-1.059049 Ha, Error=1.820 mHa

Eval 148: E=-1.059050 Ha, Error=1.818 mHa
Eval 149: E=-1.059050 Ha, Error=1.819 mHa
Eval 150: E=-1.059049 Ha, Error=1.819 mHa
Eval 151: E=-1.059049 Ha, Error=1.819 mHa
Eval 152: E=-1.059050 Ha, Error=1.819 mHa
Eval 153: E=-1.059049 Ha, Error=1.819 mHa
Eval 154: E=-1.059050 Ha, Error=1.819 mHa
Eval 155: E=-1.059049 Ha, Error=1.820 mHa
Eval 156: E=-1.059050 Ha, Error=1.818 mHa
Eval 157: E=-1.059050 Ha, Error=1.818 mHa
Eval 158: E=-1.059042 Ha, Error=1.826 mHa
Eval 159: E=-1.059050 Ha, Error=1.818 mHa
Eval 160: E=-1.059049 Ha, Error=1.819 mHa
Eval 161: E=-1.059050 Ha, Error=1.818 mHa
Eval 162: E=-1.059049 Ha, Error=1.819 mHa
Eval 163: E=-1.059050 Ha, Error=1.818 mHa
Eval 164: E=-1.059049 Ha, Error=1.819 mHa
Eval 165: E=-1.059050 Ha, Error=1.818 mHa
Eval 166: E=-1.059049 Ha, Error=1.820 mHa
Eval 167: E=-1.059050 Ha, Error=1.819 mHa
Eval 168: E=-1.059048 Ha, Error=1.820 mHa
Eval 169: E=-1.059049 Ha, Error=1.819 mHa
Eval 170: E=-1.059049 Ha, Error=1.819 mHa
Eval 171: E=-1.059049 Ha, Error=1.819 mHa
Eval 172: E=-1.059046 Ha, Error=1.822 mHa
Eval 173: E=-1.059050 Ha, Error=1.818 mHa
Eval 174: E=-1.059047 Ha, Error=1.821 mHa
Eval 175: E=-1.059050 Ha, Error=1.818 mHa
Eval 176: E=-1.059045 Ha, Error=1.823 mHa
Eval 177: E=-1.059050 Ha, Error=1.818 mHa
Eval 178: E=-1.059049 Ha, Error=1.819 mHa
Eval 179: E=-1.059050 Ha, Error=1.818 mHa
Eval 180: E=-1.059041 Ha, Error=1.827 mHa
Eval 181: E=-1.059049 Ha, Error=1.819 mHa
Eval 182: E=-1.059048 Ha, Error=1.821 mHa
Eval 183: E=-1.059050 Ha, Error=1.818 mHa
Eval 184: E=-1.059042 Ha, Error=1.826 mHa
Eval 185: E=-1.059050 Ha, Error=1.818 mHa
Eval 186: E=-1.059049 Ha, Error=1.819 mHa
Eval 187: E=-1.059048 Ha, Error=1.820 mHa
Eval 188: E=-1.059050 Ha, Error=1.818 mHa
Eval 189: E=-1.059050 Ha, Error=1.818 mHa
Eval 190: E=-1.059050 Ha, Error=1.818 mHa
Eval 191: E=-1.059050 Ha, Error=1.818 mHa
Eval 192: E=-1.059050 Ha, Error=1.818 mHa
Eval 193: E=-1.059050 Ha, Error=1.818 mHa
Eval 194: E=-1.059050 Ha, Error=1.818 mHa
Eval 195: E=-1.059050 Ha, Error=1.818 mHa


```

Eval 292: E=-1.059050 Ha, Error=1.818 mHa
Eval 293: E=-1.059050 Ha, Error=1.818 mHa
Eval 294: E=-1.059050 Ha, Error=1.818 mHa
Eval 295: E=-1.059050 Ha, Error=1.818 mHa
Eval 296: E=-1.059050 Ha, Error=1.818 mHa
Eval 297: E=-1.059050 Ha, Error=1.818 mHa
Eval 298: E=-1.059050 Ha, Error=1.818 mHa
Eval 299: E=-1.059050 Ha, Error=1.818 mHa
Eval 300: E=-1.059050 Ha, Error=1.818 mHa
VQE compute_minimum_eigenvalue took: 2.4s

```

```

Completed in 2.4s
Function evaluations: 300
Callback captured: 300 points
Energy Error: 1.817963e-03 Ha (0.1714%)
Fidelity: 0.997037
Convergence: 300/300 iterations

```

1.6 Step 6: Run All Benchmarks (Iterate Through Ansatz Dictionary)

```
[21]: # Run all benchmarks by iterating through the ansatz dictionary
all_results = []
total_benchmarks = len(ansatz_dict) * NUM_RUNS
current_benchmark = 0

print("=="*80)
print(f"STARTING COMPREHENSIVE BENCHMARK SUITE")
print(f"Total benchmarks to run: {total_benchmarks}")
print(f"Estimated time: {total_benchmarks * 3:.0f}--{total_benchmarks * 5:.0f} minutes")
print("=="*80)

benchmark_start_time = time.time()

# Iterate through the ansatz dictionary
for ansatz_name, ansatz in ansatz_dict.items():

    if ansatz_name == "QEB-4q":
        print("\n" + "=="*60)
        print(f"  QEB-4q uses a different pipeline (4-qubit projected H)")
        print(f"  Skipping in this benchmark loop, will run separately")
        print("=="*60)
        continue # Skip to next ansatz
    # =====

    for run_num in range(1, NUM_RUNS + 1):
        current_benchmark += 1

```

```

print(f"\n\n{'#' * 80}")
print(f"BENCHMARK {current_benchmark}/{total_benchmarks}")
print(f"Ansatz: {ansatz_name} | Run: {run_num}/{NUM_RUNS}")
print(f"{'#' * 80}")

# Run benchmark with the ansatz from dictionary
result = run_vqe_benchmark(
    ansatz=ansatz,
    ansatz_name=ansatz_name,
    run_number=run_num,
    qubit_op=qubit_op,
    exact_electronic=exact_electronic,
    exact_state=exact_state,
    problem=problem,
    maxiter=300
)

all_results.append(result)

# Progress update
elapsed = time.time() - benchmark_start_time
avg_time_per_run = elapsed / current_benchmark
remaining = (total_benchmarks - current_benchmark) * avg_time_per_run
print(f"\n  Progress: {current_benchmark}/{total_benchmarks} complete")
print(f"  Elapsed: {elapsed/60:.1f} min | Estimated remaining: "
      f"{remaining/60:.1f} min")

total_time = time.time() - benchmark_start_time

print(f"\n\n{'=' * 80}")
print(f"  ALL BENCHMARKS COMPLETE!")
print(f"{'=' * 80}")
print(f"Total time: {total_time/60:.1f} minutes ({total_time:.0f} seconds)")
print(f"Average time per benchmark: {total_time/total_benchmarks:.1f} seconds")
print(f"Total runs: {len(all_results)}")
print(f"Ansätze tested: {', '.join(ansatz_dict.keys())}")
print(f"{'=' * 80}\n")

```

```
=====
STARTING COMPREHENSIVE BENCHMARK SUITE
Total benchmarks to run: 15
Estimated time: 45-75 minutes
=====
```

```
#####
BENCHMARK 1/15
```

Ansatz: UCCSD | Run: 1/3

#####
=====

Running: UCCSD - Run #1

Optimizer: COBYLA (maxiter=300)

Parameters: 15, Depth: 16

=====
Starting VQE optimization now...

Eval 1: E=-1.058211 Ha, Error=2.657 mHa
Eval 2: E=-0.949848 Ha, Error=111.021 mHa
Eval 3: E=-0.916322 Ha, Error=144.546 mHa
Eval 4: E=-0.915135 Ha, Error=145.733 mHa
Eval 5: E=-0.951391 Ha, Error=109.477 mHa
Eval 6: E=-0.915127 Ha, Error=145.741 mHa
Eval 7: E=-0.916747 Ha, Error=144.121 mHa
Eval 8: E=-0.559076 Ha, Error=501.792 mHa
Eval 9: E=-0.601074 Ha, Error=459.794 mHa
Eval 10: E=-0.604744 Ha, Error=456.124 mHa
Eval 11: E=-0.612346 Ha, Error=448.522 mHa
Eval 12: E=-0.568154 Ha, Error=492.714 mHa
Eval 13: E=-0.609360 Ha, Error=451.508 mHa
Eval 14: E=-0.620164 Ha, Error=440.704 mHa
Eval 15: E=-0.616726 Ha, Error=444.142 mHa
Eval 16: E=-0.563561 Ha, Error=497.307 mHa
Eval 17: E=-0.701190 Ha, Error=359.678 mHa
Eval 18: E=-0.896241 Ha, Error=164.627 mHa
Eval 19: E=-1.031277 Ha, Error=29.591 mHa
Eval 20: E=-1.057176 Ha, Error=3.692 mHa
Eval 21: E=-1.047929 Ha, Error=12.939 mHa
Eval 22: E=-1.056876 Ha, Error=3.992 mHa
Eval 23: E=-1.048664 Ha, Error=12.204 mHa
Eval 24: E=-1.057217 Ha, Error=3.651 mHa
Eval 25: E=-1.050315 Ha, Error=10.553 mHa
Eval 26: E=-1.057499 Ha, Error=3.369 mHa
Eval 27: E=-1.050839 Ha, Error=10.030 mHa
Eval 28: E=-1.057560 Ha, Error=3.308 mHa
Eval 29: E=-1.051623 Ha, Error=9.245 mHa
Eval 30: E=-1.057525 Ha, Error=3.343 mHa
Eval 31: E=-1.052425 Ha, Error=8.443 mHa
Eval 32: E=-1.056327 Ha, Error=4.541 mHa
Eval 33: E=-1.055581 Ha, Error=5.287 mHa
Eval 34: E=-1.053980 Ha, Error=6.888 mHa
Eval 35: E=-1.057704 Ha, Error=3.164 mHa
Eval 36: E=-1.054783 Ha, Error=6.085 mHa
Eval 37: E=-1.058468 Ha, Error=2.400 mHa
Eval 38: E=-1.059532 Ha, Error=1.336 mHa
Eval 39: E=-1.058905 Ha, Error=1.963 mHa

Eval 40: E=-1.059477 Ha, Error=1.392 mHa
Eval 41: E=-1.059473 Ha, Error=1.395 mHa
Eval 42: E=-1.059485 Ha, Error=1.383 mHa
Eval 43: E=-1.059728 Ha, Error=1.140 mHa
Eval 44: E=-1.059614 Ha, Error=1.254 mHa
Eval 45: E=-1.059866 Ha, Error=1.002 mHa
Eval 46: E=-1.060255 Ha, Error=0.613 mHa
Eval 47: E=-1.060322 Ha, Error=0.546 mHa
Eval 48: E=-1.060385 Ha, Error=0.483 mHa
Eval 49: E=-1.060463 Ha, Error=0.405 mHa
Eval 50: E=-1.060356 Ha, Error=0.512 mHa
Eval 51: E=-1.060450 Ha, Error=0.418 mHa
Eval 52: E=-1.060562 Ha, Error=0.306 mHa
Eval 53: E=-1.060359 Ha, Error=0.510 mHa
Eval 54: E=-1.060546 Ha, Error=0.322 mHa
Eval 55: E=-1.060624 Ha, Error=0.244 mHa
Eval 56: E=-1.060598 Ha, Error=0.270 mHa
Eval 57: E=-1.060601 Ha, Error=0.267 mHa
Eval 58: E=-1.060660 Ha, Error=0.208 mHa
Eval 59: E=-1.060713 Ha, Error=0.155 mHa
Eval 60: E=-1.060691 Ha, Error=0.177 mHa
Eval 61: E=-1.060689 Ha, Error=0.179 mHa
Eval 62: E=-1.060687 Ha, Error=0.181 mHa
Eval 63: E=-1.060685 Ha, Error=0.184 mHa
Eval 64: E=-1.060706 Ha, Error=0.162 mHa
Eval 65: E=-1.060684 Ha, Error=0.184 mHa
Eval 66: E=-1.060652 Ha, Error=0.216 mHa
Eval 67: E=-1.060678 Ha, Error=0.190 mHa
Eval 68: E=-1.060662 Ha, Error=0.206 mHa
Eval 69: E=-1.060723 Ha, Error=0.145 mHa
Eval 70: E=-1.060659 Ha, Error=0.210 mHa
Eval 71: E=-1.060699 Ha, Error=0.169 mHa
Eval 72: E=-1.060690 Ha, Error=0.178 mHa
Eval 73: E=-1.060731 Ha, Error=0.137 mHa
Eval 74: E=-1.060731 Ha, Error=0.137 mHa
Eval 75: E=-1.060729 Ha, Error=0.139 mHa
Eval 76: E=-1.060739 Ha, Error=0.130 mHa
Eval 77: E=-1.060741 Ha, Error=0.127 mHa
Eval 78: E=-1.060746 Ha, Error=0.122 mHa
Eval 79: E=-1.060750 Ha, Error=0.119 mHa
Eval 80: E=-1.060751 Ha, Error=0.117 mHa
Eval 81: E=-1.060755 Ha, Error=0.113 mHa
Eval 82: E=-1.060758 Ha, Error=0.110 mHa
Eval 83: E=-1.060761 Ha, Error=0.107 mHa
Eval 84: E=-1.060762 Ha, Error=0.107 mHa
Eval 85: E=-1.060760 Ha, Error=0.108 mHa
Eval 86: E=-1.060758 Ha, Error=0.110 mHa
Eval 87: E=-1.060764 Ha, Error=0.104 mHa

Eval 88: E=-1.060764 Ha, Error=0.104 mHa
Eval 89: E=-1.060764 Ha, Error=0.104 mHa
Eval 90: E=-1.060763 Ha, Error=0.105 mHa
Eval 91: E=-1.060770 Ha, Error=0.098 mHa
Eval 92: E=-1.060770 Ha, Error=0.098 mHa
Eval 93: E=-1.060767 Ha, Error=0.101 mHa
Eval 94: E=-1.060779 Ha, Error=0.089 mHa
Eval 95: E=-1.060786 Ha, Error=0.083 mHa
Eval 96: E=-1.060792 Ha, Error=0.076 mHa
Eval 97: E=-1.060798 Ha, Error=0.070 mHa
Eval 98: E=-1.060802 Ha, Error=0.066 mHa
Eval 99: E=-1.060808 Ha, Error=0.060 mHa
Eval 100: E=-1.060810 Ha, Error=0.058 mHa
Eval 101: E=-1.060812 Ha, Error=0.057 mHa
Eval 102: E=-1.060814 Ha, Error=0.054 mHa
Eval 103: E=-1.060815 Ha, Error=0.053 mHa
Eval 104: E=-1.060815 Ha, Error=0.054 mHa
Eval 105: E=-1.060814 Ha, Error=0.054 mHa
Eval 106: E=-1.060817 Ha, Error=0.051 mHa
Eval 107: E=-1.060819 Ha, Error=0.049 mHa
Eval 108: E=-1.060819 Ha, Error=0.049 mHa
Eval 109: E=-1.060819 Ha, Error=0.049 mHa
Eval 110: E=-1.060818 Ha, Error=0.050 mHa
Eval 111: E=-1.060823 Ha, Error=0.045 mHa
Eval 112: E=-1.060828 Ha, Error=0.040 mHa
Eval 113: E=-1.060832 Ha, Error=0.036 mHa
Eval 114: E=-1.060833 Ha, Error=0.035 mHa
Eval 115: E=-1.060836 Ha, Error=0.032 mHa
Eval 116: E=-1.060840 Ha, Error=0.029 mHa
Eval 117: E=-1.060841 Ha, Error=0.027 mHa
Eval 118: E=-1.060841 Ha, Error=0.027 mHa
Eval 119: E=-1.060840 Ha, Error=0.028 mHa
Eval 120: E=-1.060844 Ha, Error=0.025 mHa
Eval 121: E=-1.060844 Ha, Error=0.024 mHa
Eval 122: E=-1.060846 Ha, Error=0.022 mHa
Eval 123: E=-1.060848 Ha, Error=0.020 mHa
Eval 124: E=-1.060849 Ha, Error=0.019 mHa
Eval 125: E=-1.060852 Ha, Error=0.017 mHa
Eval 126: E=-1.060852 Ha, Error=0.016 mHa
Eval 127: E=-1.060853 Ha, Error=0.015 mHa
Eval 128: E=-1.060852 Ha, Error=0.016 mHa
Eval 129: E=-1.060852 Ha, Error=0.016 mHa
Eval 130: E=-1.060854 Ha, Error=0.014 mHa
Eval 131: E=-1.060857 Ha, Error=0.012 mHa
Eval 132: E=-1.060858 Ha, Error=0.010 mHa
Eval 133: E=-1.060860 Ha, Error=0.009 mHa
Eval 134: E=-1.060861 Ha, Error=0.007 mHa
Eval 135: E=-1.060861 Ha, Error=0.007 mHa

Eval 136: E=-1.060860 Ha, Error=0.008 mHa
Eval 137: E=-1.060861 Ha, Error=0.007 mHa
Eval 138: E=-1.060862 Ha, Error=0.006 mHa
Eval 139: E=-1.060863 Ha, Error=0.005 mHa
Eval 140: E=-1.060863 Ha, Error=0.005 mHa
Eval 141: E=-1.060864 Ha, Error=0.004 mHa
Eval 142: E=-1.060864 Ha, Error=0.005 mHa
Eval 143: E=-1.060864 Ha, Error=0.004 mHa
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Eval 145: E=-1.060865 Ha, Error=0.003 mHa
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Eval 148: E=-1.060866 Ha, Error=0.002 mHa
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Eval 163: E=-1.060866 Ha, Error=0.002 mHa
Eval 164: E=-1.060867 Ha, Error=0.001 mHa
Eval 165: E=-1.060866 Ha, Error=0.002 mHa
Eval 166: E=-1.060867 Ha, Error=0.001 mHa
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Eval 168: E=-1.060867 Ha, Error=0.002 mHa
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Eval 198: E=-1.060868 Ha, Error=0.001 mHa
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Eval 203: E=-1.060868 Ha, Error=0.000 mHa
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Eval 205: E=-1.060868 Ha, Error=0.000 mHa
Eval 206: E=-1.060868 Ha, Error=0.000 mHa
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Eval 209: E=-1.060868 Ha, Error=0.000 mHa
Eval 210: E=-1.060868 Ha, Error=0.000 mHa
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Eval 230: E=-1.060868 Ha, Error=0.000 mHa
Eval 231: E=-1.060868 Ha, Error=0.000 mHa


```
Eval 280: E=-1.060868 Ha, Error=0.000 mHa
Eval 281: E=-1.060868 Ha, Error=0.000 mHa
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Eval 283: E=-1.060868 Ha, Error=0.000 mHa
Eval 284: E=-1.060868 Ha, Error=0.000 mHa
Eval 285: E=-1.060868 Ha, Error=0.000 mHa
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Eval 287: E=-1.060868 Ha, Error=0.000 mHa
Eval 288: E=-1.060868 Ha, Error=0.000 mHa
Eval 289: E=-1.060868 Ha, Error=0.000 mHa
Eval 290: E=-1.060868 Ha, Error=0.000 mHa
Eval 291: E=-1.060868 Ha, Error=0.000 mHa
Eval 292: E=-1.060868 Ha, Error=0.000 mHa
Eval 293: E=-1.060868 Ha, Error=0.000 mHa
Eval 294: E=-1.060868 Ha, Error=0.000 mHa
Eval 295: E=-1.060868 Ha, Error=0.000 mHa
Eval 296: E=-1.060868 Ha, Error=0.000 mHa
Eval 297: E=-1.060868 Ha, Error=0.000 mHa
Eval 298: E=-1.060868 Ha, Error=0.000 mHa
Eval 299: E=-1.060868 Ha, Error=0.000 mHa
Eval 300: E=-1.060868 Ha, Error=0.000 mHa
VQE compute_minimum_eigenvalue took: 72.8s
```

```
Completed in 72.8s
Function evaluations: 300
Callback captured: 300 points
Energy Error: 2.768017e-09 Ha (0.0000%)
Fidelity: 1.000000
Convergence: 119/300 iterations
```

```
Progress: 1/15 complete
Elapsed: 1.2 min | Estimated remaining: 17.0 min
```

```
#####
BENCHMARK 2/15
Ansatz: UCCSD | Run: 2/3
#####
```

```
=====
Running: UCCSD - Run #2
Optimizer: COBYLA (maxiter=300)
Parameters: 15, Depth: 16
=====
```

```
Starting VQE optimization now...
Eval 1: E=-1.058768 Ha, Error=2.100 mHa
Eval 2: E=-0.951201 Ha, Error=109.667 mHa
Eval 3: E=-0.912440 Ha, Error=148.428 mHa
```

Eval 4: E=-0.911712 Ha, Error=149.156 mHa
Eval 5: E=-0.952965 Ha, Error=107.903 mHa
Eval 6: E=-0.917100 Ha, Error=143.768 mHa
Eval 7: E=-0.917260 Ha, Error=143.609 mHa
Eval 8: E=-0.550260 Ha, Error=510.608 mHa
Eval 9: E=-0.610456 Ha, Error=450.413 mHa
Eval 10: E=-0.611650 Ha, Error=449.219 mHa
Eval 11: E=-0.609729 Ha, Error=451.140 mHa
Eval 12: E=-0.570743 Ha, Error=490.125 mHa
Eval 13: E=-0.613334 Ha, Error=447.534 mHa
Eval 14: E=-0.619821 Ha, Error=441.047 mHa
Eval 15: E=-0.608959 Ha, Error=451.909 mHa
Eval 16: E=-0.570938 Ha, Error=489.930 mHa
Eval 17: E=-0.701991 Ha, Error=358.877 mHa
Eval 18: E=-0.887526 Ha, Error=173.342 mHa
Eval 19: E=-1.031250 Ha, Error=29.618 mHa
Eval 20: E=-1.057676 Ha, Error=3.193 mHa
Eval 21: E=-1.050081 Ha, Error=10.787 mHa
Eval 22: E=-1.057810 Ha, Error=3.058 mHa
Eval 23: E=-1.049599 Ha, Error=11.270 mHa
Eval 24: E=-1.058268 Ha, Error=2.600 mHa
Eval 25: E=-1.052395 Ha, Error=8.473 mHa
Eval 26: E=-1.057924 Ha, Error=2.944 mHa
Eval 27: E=-1.052638 Ha, Error=8.230 mHa
Eval 28: E=-1.057795 Ha, Error=3.073 mHa
Eval 29: E=-1.053294 Ha, Error=7.575 mHa
Eval 30: E=-1.057822 Ha, Error=3.046 mHa
Eval 31: E=-1.053855 Ha, Error=7.014 mHa
Eval 32: E=-1.056711 Ha, Error=4.157 mHa
Eval 33: E=-1.056251 Ha, Error=4.617 mHa
Eval 34: E=-1.054361 Ha, Error=6.507 mHa
Eval 35: E=-1.055993 Ha, Error=4.875 mHa
Eval 36: E=-1.054828 Ha, Error=6.040 mHa
Eval 37: E=-1.058731 Ha, Error=2.137 mHa
Eval 38: E=-1.059563 Ha, Error=1.306 mHa
Eval 39: E=-1.058998 Ha, Error=1.870 mHa
Eval 40: E=-1.059502 Ha, Error=1.366 mHa
Eval 41: E=-1.059540 Ha, Error=1.328 mHa
Eval 42: E=-1.059522 Ha, Error=1.346 mHa
Eval 43: E=-1.059767 Ha, Error=1.101 mHa
Eval 44: E=-1.059555 Ha, Error=1.313 mHa
Eval 45: E=-1.059924 Ha, Error=0.945 mHa
Eval 46: E=-1.060278 Ha, Error=0.590 mHa
Eval 47: E=-1.060333 Ha, Error=0.535 mHa
Eval 48: E=-1.060408 Ha, Error=0.460 mHa
Eval 49: E=-1.060302 Ha, Error=0.566 mHa
Eval 50: E=-1.060413 Ha, Error=0.455 mHa
Eval 51: E=-1.060469 Ha, Error=0.400 mHa

Eval 52: E=-1.060537 Ha, Error=0.332 mHa
Eval 53: E=-1.060529 Ha, Error=0.339 mHa
Eval 54: E=-1.060553 Ha, Error=0.315 mHa
Eval 55: E=-1.060625 Ha, Error=0.243 mHa
Eval 56: E=-1.060437 Ha, Error=0.431 mHa
Eval 57: E=-1.060613 Ha, Error=0.256 mHa
Eval 58: E=-1.060618 Ha, Error=0.250 mHa
Eval 59: E=-1.060591 Ha, Error=0.277 mHa
Eval 60: E=-1.060737 Ha, Error=0.131 mHa
Eval 61: E=-1.060697 Ha, Error=0.171 mHa
Eval 62: E=-1.060705 Ha, Error=0.163 mHa
Eval 63: E=-1.060752 Ha, Error=0.116 mHa
Eval 64: E=-1.060691 Ha, Error=0.177 mHa
Eval 65: E=-1.060723 Ha, Error=0.146 mHa
Eval 66: E=-1.060722 Ha, Error=0.146 mHa
Eval 67: E=-1.060695 Ha, Error=0.173 mHa
Eval 68: E=-1.060739 Ha, Error=0.129 mHa
Eval 69: E=-1.060741 Ha, Error=0.127 mHa
Eval 70: E=-1.060706 Ha, Error=0.162 mHa
Eval 71: E=-1.060745 Ha, Error=0.124 mHa
Eval 72: E=-1.060766 Ha, Error=0.102 mHa
Eval 73: E=-1.060714 Ha, Error=0.154 mHa
Eval 74: E=-1.060735 Ha, Error=0.133 mHa
Eval 75: E=-1.060737 Ha, Error=0.131 mHa
Eval 76: E=-1.060738 Ha, Error=0.131 mHa
Eval 77: E=-1.060731 Ha, Error=0.137 mHa
Eval 78: E=-1.060749 Ha, Error=0.119 mHa
Eval 79: E=-1.060729 Ha, Error=0.139 mHa
Eval 80: E=-1.060760 Ha, Error=0.108 mHa
Eval 81: E=-1.060776 Ha, Error=0.093 mHa
Eval 82: E=-1.060777 Ha, Error=0.091 mHa
Eval 83: E=-1.060779 Ha, Error=0.089 mHa
Eval 84: E=-1.060778 Ha, Error=0.090 mHa
Eval 85: E=-1.060778 Ha, Error=0.091 mHa
Eval 86: E=-1.060784 Ha, Error=0.084 mHa
Eval 87: E=-1.060784 Ha, Error=0.084 mHa
Eval 88: E=-1.060786 Ha, Error=0.082 mHa
Eval 89: E=-1.060785 Ha, Error=0.084 mHa
Eval 90: E=-1.060786 Ha, Error=0.082 mHa
Eval 91: E=-1.060790 Ha, Error=0.078 mHa
Eval 92: E=-1.060791 Ha, Error=0.077 mHa
Eval 93: E=-1.060793 Ha, Error=0.075 mHa
Eval 94: E=-1.060794 Ha, Error=0.074 mHa
Eval 95: E=-1.060794 Ha, Error=0.074 mHa
Eval 96: E=-1.060790 Ha, Error=0.078 mHa
Eval 97: E=-1.060799 Ha, Error=0.069 mHa
Eval 98: E=-1.060806 Ha, Error=0.062 mHa
Eval 99: E=-1.060810 Ha, Error=0.058 mHa

Eval 100: E=-1.060813 Ha, Error=0.055 mHa
Eval 101: E=-1.060816 Ha, Error=0.052 mHa
Eval 102: E=-1.060817 Ha, Error=0.051 mHa
Eval 103: E=-1.060818 Ha, Error=0.050 mHa
Eval 104: E=-1.060822 Ha, Error=0.046 mHa
Eval 105: E=-1.060821 Ha, Error=0.047 mHa
Eval 106: E=-1.060820 Ha, Error=0.048 mHa
Eval 107: E=-1.060828 Ha, Error=0.040 mHa
Eval 108: E=-1.060831 Ha, Error=0.038 mHa
Eval 109: E=-1.060833 Ha, Error=0.036 mHa
Eval 110: E=-1.060837 Ha, Error=0.032 mHa
Eval 111: E=-1.060838 Ha, Error=0.030 mHa
Eval 112: E=-1.060840 Ha, Error=0.028 mHa
Eval 113: E=-1.060840 Ha, Error=0.028 mHa
Eval 114: E=-1.060839 Ha, Error=0.029 mHa
Eval 115: E=-1.060842 Ha, Error=0.026 mHa
Eval 116: E=-1.060842 Ha, Error=0.026 mHa
Eval 117: E=-1.060842 Ha, Error=0.026 mHa
Eval 118: E=-1.060842 Ha, Error=0.027 mHa
Eval 119: E=-1.060844 Ha, Error=0.024 mHa
Eval 120: E=-1.060848 Ha, Error=0.020 mHa
Eval 121: E=-1.060851 Ha, Error=0.018 mHa
Eval 122: E=-1.060852 Ha, Error=0.016 mHa
Eval 123: E=-1.060852 Ha, Error=0.016 mHa
Eval 124: E=-1.060855 Ha, Error=0.014 mHa
Eval 125: E=-1.060854 Ha, Error=0.014 mHa
Eval 126: E=-1.060854 Ha, Error=0.014 mHa
Eval 127: E=-1.060856 Ha, Error=0.012 mHa
Eval 128: E=-1.060858 Ha, Error=0.010 mHa
Eval 129: E=-1.060858 Ha, Error=0.011 mHa
Eval 130: E=-1.060858 Ha, Error=0.010 mHa
Eval 131: E=-1.060859 Ha, Error=0.009 mHa
Eval 132: E=-1.060859 Ha, Error=0.009 mHa
Eval 133: E=-1.060859 Ha, Error=0.009 mHa
Eval 134: E=-1.060860 Ha, Error=0.008 mHa
Eval 135: E=-1.060860 Ha, Error=0.008 mHa
Eval 136: E=-1.060862 Ha, Error=0.007 mHa
Eval 137: E=-1.060863 Ha, Error=0.005 mHa
Eval 138: E=-1.060864 Ha, Error=0.004 mHa
Eval 139: E=-1.060864 Ha, Error=0.004 mHa
Eval 140: E=-1.060865 Ha, Error=0.003 mHa
Eval 141: E=-1.060865 Ha, Error=0.003 mHa
Eval 142: E=-1.060865 Ha, Error=0.003 mHa
Eval 143: E=-1.060865 Ha, Error=0.003 mHa
Eval 144: E=-1.060866 Ha, Error=0.003 mHa
Eval 145: E=-1.060866 Ha, Error=0.002 mHa
Eval 146: E=-1.060866 Ha, Error=0.002 mHa
Eval 147: E=-1.060866 Ha, Error=0.002 mHa

Eval 148: E=-1.060866 Ha, Error=0.002 mHa
Eval 149: E=-1.060867 Ha, Error=0.001 mHa
Eval 150: E=-1.060866 Ha, Error=0.002 mHa
Eval 151: E=-1.060866 Ha, Error=0.002 mHa
Eval 152: E=-1.060866 Ha, Error=0.002 mHa
Eval 153: E=-1.060867 Ha, Error=0.001 mHa
Eval 154: E=-1.060867 Ha, Error=0.001 mHa
Eval 155: E=-1.060867 Ha, Error=0.002 mHa
Eval 156: E=-1.060866 Ha, Error=0.002 mHa
Eval 157: E=-1.060866 Ha, Error=0.002 mHa
Eval 158: E=-1.060867 Ha, Error=0.002 mHa
Eval 159: E=-1.060866 Ha, Error=0.002 mHa
Eval 160: E=-1.060867 Ha, Error=0.001 mHa
Eval 161: E=-1.060866 Ha, Error=0.002 mHa
Eval 162: E=-1.060866 Ha, Error=0.002 mHa
Eval 163: E=-1.060867 Ha, Error=0.001 mHa
Eval 164: E=-1.060866 Ha, Error=0.002 mHa
Eval 165: E=-1.060867 Ha, Error=0.002 mHa
Eval 166: E=-1.060867 Ha, Error=0.001 mHa
Eval 167: E=-1.060867 Ha, Error=0.001 mHa
Eval 168: E=-1.060867 Ha, Error=0.002 mHa
Eval 169: E=-1.060867 Ha, Error=0.001 mHa
Eval 170: E=-1.060867 Ha, Error=0.001 mHa
Eval 171: E=-1.060867 Ha, Error=0.001 mHa
Eval 172: E=-1.060867 Ha, Error=0.001 mHa
Eval 173: E=-1.060867 Ha, Error=0.001 mHa
Eval 174: E=-1.060867 Ha, Error=0.001 mHa
Eval 175: E=-1.060867 Ha, Error=0.001 mHa
Eval 176: E=-1.060867 Ha, Error=0.001 mHa
Eval 177: E=-1.060867 Ha, Error=0.001 mHa
Eval 178: E=-1.060867 Ha, Error=0.002 mHa
Eval 179: E=-1.060867 Ha, Error=0.001 mHa
Eval 180: E=-1.060867 Ha, Error=0.001 mHa
Eval 181: E=-1.060867 Ha, Error=0.001 mHa
Eval 182: E=-1.060867 Ha, Error=0.001 mHa
Eval 183: E=-1.060867 Ha, Error=0.001 mHa
Eval 184: E=-1.060867 Ha, Error=0.001 mHa
Eval 185: E=-1.060867 Ha, Error=0.001 mHa
Eval 186: E=-1.060867 Ha, Error=0.001 mHa
Eval 187: E=-1.060867 Ha, Error=0.001 mHa
Eval 188: E=-1.060868 Ha, Error=0.001 mHa
Eval 189: E=-1.060867 Ha, Error=0.001 mHa
Eval 190: E=-1.060867 Ha, Error=0.001 mHa
Eval 191: E=-1.060868 Ha, Error=0.001 mHa
Eval 192: E=-1.060868 Ha, Error=0.001 mHa
Eval 193: E=-1.060868 Ha, Error=0.001 mHa
Eval 194: E=-1.060868 Ha, Error=0.001 mHa
Eval 195: E=-1.060868 Ha, Error=0.001 mHa


```

Eval 292: E=-1.060868 Ha, Error=0.000 mHa
Eval 293: E=-1.060868 Ha, Error=0.000 mHa
Eval 294: E=-1.060868 Ha, Error=0.000 mHa
Eval 295: E=-1.060868 Ha, Error=0.000 mHa
Eval 296: E=-1.060868 Ha, Error=0.000 mHa
Eval 297: E=-1.060868 Ha, Error=0.000 mHa
Eval 298: E=-1.060868 Ha, Error=0.000 mHa
Eval 299: E=-1.060868 Ha, Error=0.000 mHa
Eval 300: E=-1.060868 Ha, Error=0.000 mHa
VQE compute_minimum_eigenvalue took: 72.5s

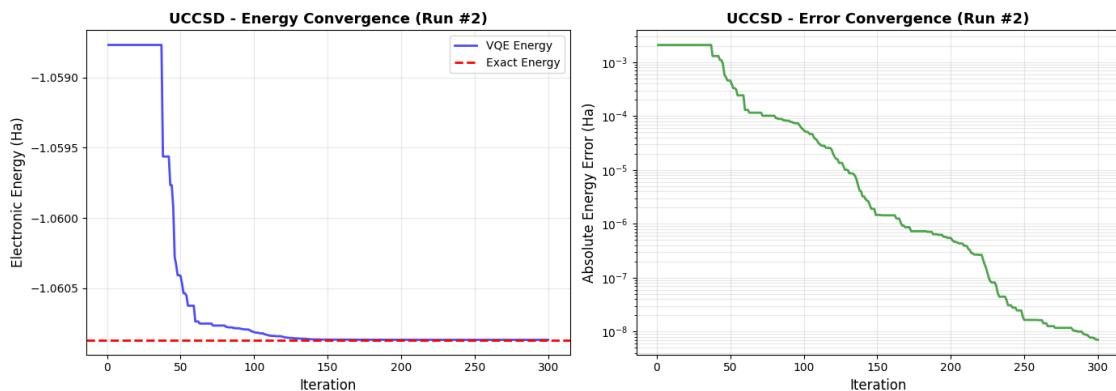
```

```

Completed in 72.5s
Function evaluations: 300
Callback captured: 300 points
Energy Error: 7.006242e-09 Ha (0.0000%)
Fidelity: 1.000000
Convergence: 119/300 iterations

```

```
*****
PLOTTING CONVERGENCE FOR UCCSD - RUN #2
*****
```



Convergence plot saved: convergence_UCCSD_run2.png

```

Progress: 2/15 complete
Elapsed: 2.4 min | Estimated remaining: 15.8 min

```

```
#####
BENCHMARK 3/15
Ansatz: UCCSD | Run: 3/3
#####
```

```
=====
Running: UCCSD - Run #3
Optimizer: COBYLA (maxiter=300)
Parameters: 15, Depth: 16
=====
```

```
Starting VQE optimization now...
Eval 1: E=-1.059153 Ha, Error=1.715 mHa
Eval 2: E=-0.950025 Ha, Error=110.843 mHa
Eval 3: E=-0.915577 Ha, Error=145.291 mHa
Eval 4: E=-0.916106 Ha, Error=144.762 mHa
Eval 5: E=-0.950678 Ha, Error=110.191 mHa
Eval 6: E=-0.917594 Ha, Error=143.274 mHa
Eval 7: E=-0.920540 Ha, Error=140.328 mHa
Eval 8: E=-0.561608 Ha, Error=499.260 mHa
Eval 9: E=-0.615884 Ha, Error=444.984 mHa
Eval 10: E=-0.608076 Ha, Error=452.793 mHa
Eval 11: E=-0.607376 Ha, Error=453.492 mHa
Eval 12: E=-0.567237 Ha, Error=493.631 mHa
Eval 13: E=-0.610710 Ha, Error=450.158 mHa
Eval 14: E=-0.619346 Ha, Error=441.523 mHa
Eval 15: E=-0.607621 Ha, Error=453.247 mHa
Eval 16: E=-0.576976 Ha, Error=483.892 mHa
Eval 17: E=-0.700519 Ha, Error=360.349 mHa
Eval 18: E=-0.897590 Ha, Error=163.278 mHa
Eval 19: E=-1.056914 Ha, Error=3.954 mHa
Eval 20: E=-1.028392 Ha, Error=32.476 mHa
Eval 21: E=-1.057852 Ha, Error=3.016 mHa
Eval 22: E=-1.049351 Ha, Error=11.517 mHa
Eval 23: E=-1.058088 Ha, Error=2.780 mHa
Eval 24: E=-1.051176 Ha, Error=9.692 mHa
Eval 25: E=-1.058568 Ha, Error=2.300 mHa
Eval 26: E=-1.052281 Ha, Error=8.587 mHa
Eval 27: E=-1.058187 Ha, Error=2.681 mHa
Eval 28: E=-1.052435 Ha, Error=8.433 mHa
Eval 29: E=-1.057873 Ha, Error=2.995 mHa
Eval 30: E=-1.053218 Ha, Error=7.651 mHa
Eval 31: E=-1.057137 Ha, Error=3.731 mHa
Eval 32: E=-1.053284 Ha, Error=7.585 mHa
Eval 33: E=-1.058781 Ha, Error=2.087 mHa
Eval 34: E=-1.054443 Ha, Error=6.425 mHa
Eval 35: E=-1.057393 Ha, Error=3.475 mHa
Eval 36: E=-1.058433 Ha, Error=2.435 mHa
Eval 37: E=-1.059185 Ha, Error=1.683 mHa
Eval 38: E=-1.059963 Ha, Error=0.905 mHa
Eval 39: E=-1.059724 Ha, Error=1.144 mHa
Eval 40: E=-1.059930 Ha, Error=0.939 mHa
Eval 41: E=-1.059874 Ha, Error=0.994 mHa
```

Eval 42: E=-1.059937 Ha, Error=0.931 mHa
Eval 43: E=-1.059962 Ha, Error=0.906 mHa
Eval 44: E=-1.059992 Ha, Error=0.876 mHa
Eval 45: E=-1.060095 Ha, Error=0.773 mHa
Eval 46: E=-1.060130 Ha, Error=0.738 mHa
Eval 47: E=-1.060051 Ha, Error=0.817 mHa
Eval 48: E=-1.060133 Ha, Error=0.736 mHa
Eval 49: E=-1.060061 Ha, Error=0.807 mHa
Eval 50: E=-1.060138 Ha, Error=0.730 mHa
Eval 51: E=-1.060101 Ha, Error=0.768 mHa
Eval 52: E=-1.060021 Ha, Error=0.847 mHa
Eval 53: E=-1.060254 Ha, Error=0.614 mHa
Eval 54: E=-1.060161 Ha, Error=0.707 mHa
Eval 55: E=-1.060203 Ha, Error=0.665 mHa
Eval 56: E=-1.060195 Ha, Error=0.673 mHa
Eval 57: E=-1.060282 Ha, Error=0.586 mHa
Eval 58: E=-1.060512 Ha, Error=0.356 mHa
Eval 59: E=-1.060516 Ha, Error=0.352 mHa
Eval 60: E=-1.060502 Ha, Error=0.366 mHa
Eval 61: E=-1.060460 Ha, Error=0.409 mHa
Eval 62: E=-1.060512 Ha, Error=0.356 mHa
Eval 63: E=-1.060488 Ha, Error=0.381 mHa
Eval 64: E=-1.060608 Ha, Error=0.260 mHa
Eval 65: E=-1.060509 Ha, Error=0.360 mHa
Eval 66: E=-1.060611 Ha, Error=0.257 mHa
Eval 67: E=-1.060604 Ha, Error=0.264 mHa
Eval 68: E=-1.060562 Ha, Error=0.306 mHa
Eval 69: E=-1.060600 Ha, Error=0.268 mHa
Eval 70: E=-1.060613 Ha, Error=0.255 mHa
Eval 71: E=-1.060574 Ha, Error=0.294 mHa
Eval 72: E=-1.060602 Ha, Error=0.266 mHa
Eval 73: E=-1.060581 Ha, Error=0.287 mHa
Eval 74: E=-1.060580 Ha, Error=0.288 mHa
Eval 75: E=-1.060632 Ha, Error=0.236 mHa
Eval 76: E=-1.060585 Ha, Error=0.283 mHa
Eval 77: E=-1.060562 Ha, Error=0.306 mHa
Eval 78: E=-1.060636 Ha, Error=0.232 mHa
Eval 79: E=-1.060671 Ha, Error=0.197 mHa
Eval 80: E=-1.060560 Ha, Error=0.308 mHa
Eval 81: E=-1.060667 Ha, Error=0.201 mHa
Eval 82: E=-1.060619 Ha, Error=0.249 mHa
Eval 83: E=-1.060621 Ha, Error=0.247 mHa
Eval 84: E=-1.060675 Ha, Error=0.193 mHa
Eval 85: E=-1.060655 Ha, Error=0.213 mHa
Eval 86: E=-1.060652 Ha, Error=0.216 mHa
Eval 87: E=-1.060741 Ha, Error=0.128 mHa
Eval 88: E=-1.060707 Ha, Error=0.161 mHa
Eval 89: E=-1.060727 Ha, Error=0.141 mHa

Eval 90: E=-1.060648 Ha, Error=0.221 mHa
Eval 91: E=-1.060743 Ha, Error=0.125 mHa
Eval 92: E=-1.060688 Ha, Error=0.181 mHa
Eval 93: E=-1.060741 Ha, Error=0.127 mHa
Eval 94: E=-1.060718 Ha, Error=0.151 mHa
Eval 95: E=-1.060725 Ha, Error=0.144 mHa
Eval 96: E=-1.060700 Ha, Error=0.168 mHa
Eval 97: E=-1.060713 Ha, Error=0.155 mHa
Eval 98: E=-1.060709 Ha, Error=0.159 mHa
Eval 99: E=-1.060736 Ha, Error=0.132 mHa
Eval 100: E=-1.060733 Ha, Error=0.135 mHa
Eval 101: E=-1.060747 Ha, Error=0.122 mHa
Eval 102: E=-1.060744 Ha, Error=0.124 mHa
Eval 103: E=-1.060748 Ha, Error=0.120 mHa
Eval 104: E=-1.060755 Ha, Error=0.113 mHa
Eval 105: E=-1.060758 Ha, Error=0.110 mHa
Eval 106: E=-1.060758 Ha, Error=0.110 mHa
Eval 107: E=-1.060757 Ha, Error=0.111 mHa
Eval 108: E=-1.060764 Ha, Error=0.104 mHa
Eval 109: E=-1.060770 Ha, Error=0.099 mHa
Eval 110: E=-1.060776 Ha, Error=0.092 mHa
Eval 111: E=-1.060780 Ha, Error=0.088 mHa
Eval 112: E=-1.060784 Ha, Error=0.084 mHa
Eval 113: E=-1.060786 Ha, Error=0.082 mHa
Eval 114: E=-1.060788 Ha, Error=0.080 mHa
Eval 115: E=-1.060790 Ha, Error=0.078 mHa
Eval 116: E=-1.060791 Ha, Error=0.077 mHa
Eval 117: E=-1.060791 Ha, Error=0.077 mHa
Eval 118: E=-1.060791 Ha, Error=0.078 mHa
Eval 119: E=-1.060788 Ha, Error=0.080 mHa
Eval 120: E=-1.060794 Ha, Error=0.074 mHa
Eval 121: E=-1.060795 Ha, Error=0.073 mHa
Eval 122: E=-1.060799 Ha, Error=0.070 mHa
Eval 123: E=-1.060798 Ha, Error=0.070 mHa
Eval 124: E=-1.060797 Ha, Error=0.071 mHa
Eval 125: E=-1.060803 Ha, Error=0.065 mHa
Eval 126: E=-1.060803 Ha, Error=0.065 mHa
Eval 127: E=-1.060802 Ha, Error=0.066 mHa
Eval 128: E=-1.060811 Ha, Error=0.057 mHa
Eval 129: E=-1.060818 Ha, Error=0.051 mHa
Eval 130: E=-1.060825 Ha, Error=0.044 mHa
Eval 131: E=-1.060833 Ha, Error=0.035 mHa
Eval 132: E=-1.060841 Ha, Error=0.027 mHa
Eval 133: E=-1.060842 Ha, Error=0.026 mHa
Eval 134: E=-1.060844 Ha, Error=0.025 mHa
Eval 135: E=-1.060846 Ha, Error=0.022 mHa
Eval 136: E=-1.060845 Ha, Error=0.023 mHa
Eval 137: E=-1.060847 Ha, Error=0.022 mHa

Eval 138: E=-1.060847 Ha, Error=0.021 mHa
Eval 139: E=-1.060847 Ha, Error=0.021 mHa
Eval 140: E=-1.060848 Ha, Error=0.021 mHa
Eval 141: E=-1.060845 Ha, Error=0.023 mHa
Eval 142: E=-1.060847 Ha, Error=0.021 mHa
Eval 143: E=-1.060848 Ha, Error=0.020 mHa
Eval 144: E=-1.060848 Ha, Error=0.020 mHa
Eval 145: E=-1.060849 Ha, Error=0.019 mHa
Eval 146: E=-1.060853 Ha, Error=0.015 mHa
Eval 147: E=-1.060854 Ha, Error=0.014 mHa
Eval 148: E=-1.060856 Ha, Error=0.012 mHa
Eval 149: E=-1.060858 Ha, Error=0.011 mHa
Eval 150: E=-1.060858 Ha, Error=0.010 mHa
Eval 151: E=-1.060859 Ha, Error=0.009 mHa
Eval 152: E=-1.060860 Ha, Error=0.009 mHa
Eval 153: E=-1.060860 Ha, Error=0.008 mHa
Eval 154: E=-1.060861 Ha, Error=0.007 mHa
Eval 155: E=-1.060859 Ha, Error=0.009 mHa
Eval 156: E=-1.060861 Ha, Error=0.007 mHa
Eval 157: E=-1.060862 Ha, Error=0.007 mHa
Eval 158: E=-1.060863 Ha, Error=0.006 mHa
Eval 159: E=-1.060862 Ha, Error=0.006 mHa
Eval 160: E=-1.060862 Ha, Error=0.006 mHa
Eval 161: E=-1.060863 Ha, Error=0.005 mHa
Eval 162: E=-1.060864 Ha, Error=0.004 mHa
Eval 163: E=-1.060864 Ha, Error=0.004 mHa
Eval 164: E=-1.060865 Ha, Error=0.004 mHa
Eval 165: E=-1.060866 Ha, Error=0.002 mHa
Eval 166: E=-1.060866 Ha, Error=0.002 mHa
Eval 167: E=-1.060866 Ha, Error=0.002 mHa
Eval 168: E=-1.060866 Ha, Error=0.002 mHa
Eval 169: E=-1.060866 Ha, Error=0.002 mHa
Eval 170: E=-1.060866 Ha, Error=0.002 mHa
Eval 171: E=-1.060866 Ha, Error=0.002 mHa
Eval 172: E=-1.060866 Ha, Error=0.003 mHa
Eval 173: E=-1.060867 Ha, Error=0.002 mHa
Eval 174: E=-1.060866 Ha, Error=0.002 mHa
Eval 175: E=-1.060867 Ha, Error=0.002 mHa
Eval 176: E=-1.060867 Ha, Error=0.001 mHa
Eval 177: E=-1.060866 Ha, Error=0.002 mHa
Eval 178: E=-1.060866 Ha, Error=0.002 mHa
Eval 179: E=-1.060867 Ha, Error=0.001 mHa
Eval 180: E=-1.060867 Ha, Error=0.001 mHa
Eval 181: E=-1.060866 Ha, Error=0.002 mHa
Eval 182: E=-1.060867 Ha, Error=0.001 mHa
Eval 183: E=-1.060867 Ha, Error=0.001 mHa
Eval 184: E=-1.060867 Ha, Error=0.001 mHa
Eval 185: E=-1.060867 Ha, Error=0.001 mHa

Eval 186: E=-1.060867 Ha, Error=0.001 mHa
Eval 187: E=-1.060867 Ha, Error=0.002 mHa
Eval 188: E=-1.060867 Ha, Error=0.001 mHa
Eval 189: E=-1.060867 Ha, Error=0.001 mHa
Eval 190: E=-1.060868 Ha, Error=0.001 mHa
Eval 191: E=-1.060868 Ha, Error=0.001 mHa
Eval 192: E=-1.060868 Ha, Error=0.000 mHa
Eval 193: E=-1.060867 Ha, Error=0.001 mHa
Eval 194: E=-1.060868 Ha, Error=0.000 mHa
Eval 195: E=-1.060868 Ha, Error=0.001 mHa
Eval 196: E=-1.060868 Ha, Error=0.000 mHa
Eval 197: E=-1.060868 Ha, Error=0.000 mHa
Eval 198: E=-1.060868 Ha, Error=0.000 mHa
Eval 199: E=-1.060868 Ha, Error=0.000 mHa
Eval 200: E=-1.060868 Ha, Error=0.000 mHa
Eval 201: E=-1.060868 Ha, Error=0.000 mHa
Eval 202: E=-1.060868 Ha, Error=0.000 mHa
Eval 203: E=-1.060868 Ha, Error=0.000 mHa
Eval 204: E=-1.060868 Ha, Error=0.000 mHa
Eval 205: E=-1.060868 Ha, Error=0.000 mHa
Eval 206: E=-1.060868 Ha, Error=0.000 mHa
Eval 207: E=-1.060868 Ha, Error=0.000 mHa
Eval 208: E=-1.060868 Ha, Error=0.000 mHa
Eval 209: E=-1.060868 Ha, Error=0.000 mHa
Eval 210: E=-1.060868 Ha, Error=0.000 mHa
Eval 211: E=-1.060868 Ha, Error=0.000 mHa
Eval 212: E=-1.060868 Ha, Error=0.000 mHa
Eval 213: E=-1.060868 Ha, Error=0.000 mHa
Eval 214: E=-1.060868 Ha, Error=0.000 mHa
Eval 215: E=-1.060868 Ha, Error=0.000 mHa
Eval 216: E=-1.060868 Ha, Error=0.000 mHa
Eval 217: E=-1.060868 Ha, Error=0.000 mHa
Eval 218: E=-1.060868 Ha, Error=0.000 mHa
Eval 219: E=-1.060868 Ha, Error=0.000 mHa
Eval 220: E=-1.060868 Ha, Error=0.000 mHa
Eval 221: E=-1.060868 Ha, Error=0.000 mHa
Eval 222: E=-1.060868 Ha, Error=0.000 mHa
Eval 223: E=-1.060868 Ha, Error=0.000 mHa
Eval 224: E=-1.060868 Ha, Error=0.000 mHa
Eval 225: E=-1.060868 Ha, Error=0.000 mHa
Eval 226: E=-1.060868 Ha, Error=0.000 mHa
Eval 227: E=-1.060868 Ha, Error=0.000 mHa
Eval 228: E=-1.060868 Ha, Error=0.000 mHa
Eval 229: E=-1.060868 Ha, Error=0.000 mHa
Eval 230: E=-1.060868 Ha, Error=0.000 mHa
Eval 231: E=-1.060868 Ha, Error=0.000 mHa
Eval 232: E=-1.060868 Ha, Error=0.000 mHa
Eval 233: E=-1.060868 Ha, Error=0.000 mHa


```
Eval 282: E=-1.060868 Ha, Error=0.000 mHa
Eval 283: E=-1.060868 Ha, Error=0.000 mHa
Eval 284: E=-1.060868 Ha, Error=0.000 mHa
Eval 285: E=-1.060868 Ha, Error=0.000 mHa
Eval 286: E=-1.060868 Ha, Error=0.000 mHa
Eval 287: E=-1.060868 Ha, Error=0.000 mHa
Eval 288: E=-1.060868 Ha, Error=0.000 mHa
Eval 289: E=-1.060868 Ha, Error=0.000 mHa
Eval 290: E=-1.060868 Ha, Error=0.000 mHa
Eval 291: E=-1.060868 Ha, Error=0.000 mHa
Eval 292: E=-1.060868 Ha, Error=0.000 mHa
Eval 293: E=-1.060868 Ha, Error=0.000 mHa
Eval 294: E=-1.060868 Ha, Error=0.000 mHa
Eval 295: E=-1.060868 Ha, Error=0.000 mHa
Eval 296: E=-1.060868 Ha, Error=0.000 mHa
Eval 297: E=-1.060868 Ha, Error=0.000 mHa
Eval 298: E=-1.060868 Ha, Error=0.000 mHa
Eval 299: E=-1.060868 Ha, Error=0.000 mHa
Eval 300: E=-1.060868 Ha, Error=0.000 mHa
VQE compute_minimum_eigenvalue took: 72.2s
```

```
Completed in 72.2s
Function evaluations: 300
Callback captured: 300 points
Energy Error: 3.302834e-09 Ha (0.0000%)
Fidelity: 1.000000
Convergence: 145/300 iterations
```

```
Progress: 3/15 complete
Elapsed: 3.6 min | Estimated remaining: 14.6 min
```

```
#####
BENCHMARK 4/15
Ansatz: UpCCGSD | Run: 1/3
#####

=====
Running: UpCCGSD - Run #1
Optimizer: COBYLA (maxiter=300)
Parameters: 36, Depth: 37
=====

Starting VQE optimization now...
Eval 1: E=-1.059032 Ha, Error=1.836 mHa
Eval 2: E=-0.916989 Ha, Error=143.879 mHa
Eval 3: E=-1.059032 Ha, Error=1.836 mHa
Eval 4: E=-1.059032 Ha, Error=1.836 mHa
Eval 5: E=-1.059025 Ha, Error=1.843 mHa
```

Eval 6: E=-1.059032 Ha, Error=1.836 mHa
Eval 7: E=-1.059032 Ha, Error=1.836 mHa
Eval 8: E=-0.931182 Ha, Error=129.686 mHa
Eval 9: E=-1.059032 Ha, Error=1.836 mHa
Eval 10: E=-1.059032 Ha, Error=1.836 mHa
Eval 11: E=-0.931818 Ha, Error=129.050 mHa
Eval 12: E=-1.059032 Ha, Error=1.836 mHa
Eval 13: E=-1.059032 Ha, Error=1.836 mHa
Eval 14: E=-1.059040 Ha, Error=1.828 mHa
Eval 15: E=-1.059040 Ha, Error=1.828 mHa
Eval 16: E=-1.059040 Ha, Error=1.828 mHa
Eval 17: E=-0.916313 Ha, Error=144.555 mHa
Eval 18: E=-1.059040 Ha, Error=1.828 mHa
Eval 19: E=-1.059040 Ha, Error=1.828 mHa
Eval 20: E=-0.916584 Ha, Error=144.284 mHa
Eval 21: E=-1.059040 Ha, Error=1.828 mHa
Eval 22: E=-1.059040 Ha, Error=1.828 mHa
Eval 23: E=-1.059048 Ha, Error=1.820 mHa
Eval 24: E=-1.059048 Ha, Error=1.820 mHa
Eval 25: E=-1.059048 Ha, Error=1.820 mHa
Eval 26: E=-0.932675 Ha, Error=128.193 mHa
Eval 27: E=-1.059048 Ha, Error=1.820 mHa
Eval 28: E=-1.059048 Ha, Error=1.820 mHa
Eval 29: E=-0.932197 Ha, Error=128.671 mHa
Eval 30: E=-1.059048 Ha, Error=1.820 mHa
Eval 31: E=-1.059048 Ha, Error=1.820 mHa
Eval 32: E=-1.059047 Ha, Error=1.821 mHa
Eval 33: E=-1.059048 Ha, Error=1.820 mHa
Eval 34: E=-1.059048 Ha, Error=1.820 mHa
Eval 35: E=-0.915812 Ha, Error=145.056 mHa
Eval 36: E=-1.059048 Ha, Error=1.820 mHa
Eval 37: E=-1.059048 Ha, Error=1.820 mHa
Eval 38: E=-0.624660 Ha, Error=436.208 mHa
Eval 39: E=-1.054991 Ha, Error=5.877 mHa
Eval 40: E=-1.056049 Ha, Error=4.819 mHa
Eval 41: E=-1.024897 Ha, Error=35.971 mHa
Eval 42: E=-1.059036 Ha, Error=1.832 mHa
Eval 43: E=-1.057715 Ha, Error=3.153 mHa
Eval 44: E=-1.059048 Ha, Error=1.820 mHa
Eval 45: E=-1.058256 Ha, Error=2.612 mHa
Eval 46: E=-1.059048 Ha, Error=1.820 mHa
Eval 47: E=-1.058059 Ha, Error=2.810 mHa
Eval 48: E=-1.059048 Ha, Error=1.820 mHa
Eval 49: E=-1.057792 Ha, Error=3.076 mHa
Eval 50: E=-1.059048 Ha, Error=1.820 mHa
Eval 51: E=-1.056907 Ha, Error=3.961 mHa
Eval 52: E=-1.059048 Ha, Error=1.820 mHa
Eval 53: E=-1.056883 Ha, Error=3.985 mHa

Eval 54: E=-1.059048 Ha, Error=1.820 mHa
Eval 55: E=-1.056081 Ha, Error=4.787 mHa
Eval 56: E=-1.059048 Ha, Error=1.820 mHa
Eval 57: E=-1.054841 Ha, Error=6.027 mHa
Eval 58: E=-1.059048 Ha, Error=1.820 mHa
Eval 59: E=-1.058942 Ha, Error=1.926 mHa
Eval 60: E=-1.059048 Ha, Error=1.820 mHa
Eval 61: E=-1.054873 Ha, Error=5.995 mHa
Eval 62: E=-1.059048 Ha, Error=1.820 mHa
Eval 63: E=-1.056702 Ha, Error=4.166 mHa
Eval 64: E=-1.059048 Ha, Error=1.820 mHa
Eval 65: E=-1.054763 Ha, Error=6.105 mHa
Eval 66: E=-1.059048 Ha, Error=1.820 mHa
Eval 67: E=-1.056755 Ha, Error=4.113 mHa
Eval 68: E=-1.059048 Ha, Error=1.820 mHa
Eval 69: E=-1.054754 Ha, Error=6.114 mHa
Eval 70: E=-1.059048 Ha, Error=1.820 mHa
Eval 71: E=-1.056759 Ha, Error=4.109 mHa
Eval 72: E=-1.059048 Ha, Error=1.820 mHa
Eval 73: E=-1.054753 Ha, Error=6.115 mHa
Eval 74: E=-1.059048 Ha, Error=1.820 mHa
Eval 75: E=-1.056759 Ha, Error=4.109 mHa
Eval 76: E=-1.059048 Ha, Error=1.820 mHa
Eval 77: E=-1.054753 Ha, Error=6.115 mHa
Eval 78: E=-1.059048 Ha, Error=1.820 mHa
Eval 79: E=-1.056759 Ha, Error=4.109 mHa
Eval 80: E=-1.059048 Ha, Error=1.820 mHa
Eval 81: E=-1.054753 Ha, Error=6.115 mHa
Eval 82: E=-1.059048 Ha, Error=1.820 mHa
Eval 83: E=-1.056759 Ha, Error=4.109 mHa
Eval 84: E=-1.059048 Ha, Error=1.820 mHa
Eval 85: E=-1.054753 Ha, Error=6.115 mHa
Eval 86: E=-1.059048 Ha, Error=1.820 mHa
Eval 87: E=-1.056778 Ha, Error=4.091 mHa
Eval 88: E=-1.059048 Ha, Error=1.820 mHa
Eval 89: E=-1.059029 Ha, Error=1.839 mHa
Eval 90: E=-1.059048 Ha, Error=1.820 mHa
Eval 91: E=-1.054861 Ha, Error=6.007 mHa
Eval 92: E=-1.059048 Ha, Error=1.820 mHa
Eval 93: E=-1.056735 Ha, Error=4.133 mHa
Eval 94: E=-1.059048 Ha, Error=1.820 mHa
Eval 95: E=-1.055112 Ha, Error=5.756 mHa
Eval 96: E=-1.058512 Ha, Error=2.356 mHa
Eval 97: E=-1.059011 Ha, Error=1.857 mHa
Eval 98: E=-1.058858 Ha, Error=2.010 mHa
Eval 99: E=-1.059046 Ha, Error=1.822 mHa
Eval 100: E=-1.059024 Ha, Error=1.844 mHa
Eval 101: E=-1.059044 Ha, Error=1.824 mHa

Eval 102: E=-1.059026 Ha, Error=1.842 mHa
Eval 103: E=-1.059047 Ha, Error=1.821 mHa
Eval 104: E=-1.059026 Ha, Error=1.843 mHa
Eval 105: E=-1.059048 Ha, Error=1.820 mHa
Eval 106: E=-1.059039 Ha, Error=1.829 mHa
Eval 107: E=-1.059048 Ha, Error=1.820 mHa
Eval 108: E=-1.059022 Ha, Error=1.846 mHa
Eval 109: E=-1.059048 Ha, Error=1.820 mHa
Eval 110: E=-1.059043 Ha, Error=1.826 mHa
Eval 111: E=-1.059048 Ha, Error=1.820 mHa
Eval 112: E=-1.059025 Ha, Error=1.844 mHa
Eval 113: E=-1.059048 Ha, Error=1.820 mHa
Eval 114: E=-1.059050 Ha, Error=1.819 mHa
Eval 115: E=-1.059049 Ha, Error=1.819 mHa
Eval 116: E=-1.059050 Ha, Error=1.819 mHa
Eval 117: E=-1.059035 Ha, Error=1.833 mHa
Eval 118: E=-1.059050 Ha, Error=1.819 mHa
Eval 119: E=-1.059037 Ha, Error=1.831 mHa
Eval 120: E=-1.059050 Ha, Error=1.819 mHa
Eval 121: E=-1.059013 Ha, Error=1.855 mHa
Eval 122: E=-1.059050 Ha, Error=1.819 mHa
Eval 123: E=-1.059028 Ha, Error=1.840 mHa
Eval 124: E=-1.059050 Ha, Error=1.819 mHa
Eval 125: E=-1.059025 Ha, Error=1.843 mHa
Eval 126: E=-1.059050 Ha, Error=1.819 mHa
Eval 127: E=-1.059018 Ha, Error=1.850 mHa
Eval 128: E=-1.059050 Ha, Error=1.819 mHa
Eval 129: E=-1.059013 Ha, Error=1.856 mHa
Eval 130: E=-1.059050 Ha, Error=1.819 mHa
Eval 131: E=-1.059034 Ha, Error=1.834 mHa
Eval 132: E=-1.059050 Ha, Error=1.819 mHa
Eval 133: E=-1.059028 Ha, Error=1.840 mHa
Eval 134: E=-1.059050 Ha, Error=1.819 mHa
Eval 135: E=-1.059018 Ha, Error=1.850 mHa
Eval 136: E=-1.059050 Ha, Error=1.819 mHa
Eval 137: E=-1.059025 Ha, Error=1.843 mHa
Eval 138: E=-1.059050 Ha, Error=1.819 mHa
Eval 139: E=-1.059013 Ha, Error=1.855 mHa
Eval 140: E=-1.059050 Ha, Error=1.819 mHa
Eval 141: E=-1.059047 Ha, Error=1.821 mHa
Eval 142: E=-1.059050 Ha, Error=1.819 mHa
Eval 143: E=-1.059043 Ha, Error=1.825 mHa
Eval 144: E=-1.059050 Ha, Error=1.819 mHa
Eval 145: E=-1.059042 Ha, Error=1.826 mHa
Eval 146: E=-1.059050 Ha, Error=1.819 mHa
Eval 147: E=-1.059019 Ha, Error=1.849 mHa
Eval 148: E=-1.059050 Ha, Error=1.819 mHa
Eval 149: E=-1.059013 Ha, Error=1.855 mHa

Eval 150: E=-1.059050 Ha, Error=1.818 mHa
Eval 151: E=-1.059036 Ha, Error=1.832 mHa
Eval 152: E=-1.059050 Ha, Error=1.818 mHa
Eval 153: E=-1.059025 Ha, Error=1.843 mHa
Eval 154: E=-1.059050 Ha, Error=1.818 mHa
Eval 155: E=-1.059028 Ha, Error=1.840 mHa
Eval 156: E=-1.059050 Ha, Error=1.818 mHa
Eval 157: E=-1.059035 Ha, Error=1.833 mHa
Eval 158: E=-1.059050 Ha, Error=1.818 mHa
Eval 159: E=-1.059021 Ha, Error=1.847 mHa
Eval 160: E=-1.059049 Ha, Error=1.819 mHa
Eval 161: E=-1.059015 Ha, Error=1.853 mHa
Eval 162: E=-1.059049 Ha, Error=1.819 mHa
Eval 163: E=-1.059027 Ha, Error=1.841 mHa
Eval 164: E=-1.059049 Ha, Error=1.819 mHa
Eval 165: E=-1.059029 Ha, Error=1.840 mHa
Eval 166: E=-1.059050 Ha, Error=1.818 mHa
Eval 167: E=-1.059036 Ha, Error=1.832 mHa
Eval 168: E=-1.059050 Ha, Error=1.818 mHa
Eval 169: E=-1.059015 Ha, Error=1.853 mHa
Eval 170: E=-1.059049 Ha, Error=1.820 mHa
Eval 171: E=-1.059022 Ha, Error=1.846 mHa
Eval 172: E=-1.059050 Ha, Error=1.818 mHa
Eval 173: E=-1.059016 Ha, Error=1.853 mHa
Eval 174: E=-1.059050 Ha, Error=1.818 mHa
Eval 175: E=-1.059022 Ha, Error=1.846 mHa
Eval 176: E=-1.059050 Ha, Error=1.818 mHa
Eval 177: E=-1.059047 Ha, Error=1.821 mHa
Eval 178: E=-1.059050 Ha, Error=1.818 mHa
Eval 179: E=-1.059016 Ha, Error=1.852 mHa
Eval 180: E=-1.059050 Ha, Error=1.818 mHa
Eval 181: E=-1.059023 Ha, Error=1.845 mHa
Eval 182: E=-1.059050 Ha, Error=1.818 mHa
Eval 183: E=-1.059027 Ha, Error=1.841 mHa
Eval 184: E=-1.059050 Ha, Error=1.818 mHa
Eval 185: E=-1.059047 Ha, Error=1.821 mHa
Eval 186: E=-1.059050 Ha, Error=1.818 mHa
Eval 187: E=-1.059029 Ha, Error=1.839 mHa
Eval 188: E=-1.059050 Ha, Error=1.818 mHa
Eval 189: E=-1.059035 Ha, Error=1.833 mHa
Eval 190: E=-1.059050 Ha, Error=1.818 mHa
Eval 191: E=-1.059014 Ha, Error=1.854 mHa
Eval 192: E=-1.059050 Ha, Error=1.818 mHa
Eval 193: E=-1.059027 Ha, Error=1.841 mHa
Eval 194: E=-1.059050 Ha, Error=1.818 mHa
Eval 195: E=-1.059023 Ha, Error=1.845 mHa
Eval 196: E=-1.059048 Ha, Error=1.820 mHa
Eval 197: E=-1.059035 Ha, Error=1.833 mHa

Eval 198: E=-1.059050 Ha, Error=1.818 mHa
Eval 199: E=-1.059043 Ha, Error=1.825 mHa
Eval 200: E=-1.059050 Ha, Error=1.818 mHa
Eval 201: E=-1.059032 Ha, Error=1.836 mHa
Eval 202: E=-1.059050 Ha, Error=1.818 mHa
Eval 203: E=-1.059013 Ha, Error=1.855 mHa
Eval 204: E=-1.059050 Ha, Error=1.818 mHa
Eval 205: E=-1.059048 Ha, Error=1.820 mHa
Eval 206: E=-1.059050 Ha, Error=1.818 mHa
Eval 207: E=-1.059048 Ha, Error=1.820 mHa
Eval 208: E=-1.059050 Ha, Error=1.818 mHa
Eval 209: E=-1.059016 Ha, Error=1.853 mHa
Eval 210: E=-1.059050 Ha, Error=1.818 mHa
Eval 211: E=-1.059025 Ha, Error=1.843 mHa
Eval 212: E=-1.059050 Ha, Error=1.818 mHa
Eval 213: E=-1.059028 Ha, Error=1.840 mHa
Eval 214: E=-1.059050 Ha, Error=1.818 mHa
Eval 215: E=-1.059035 Ha, Error=1.833 mHa
Eval 216: E=-1.059050 Ha, Error=1.819 mHa
Eval 217: E=-1.059015 Ha, Error=1.853 mHa
Eval 218: E=-1.059050 Ha, Error=1.818 mHa
Eval 219: E=-1.059033 Ha, Error=1.836 mHa
Eval 220: E=-1.059050 Ha, Error=1.818 mHa
Eval 221: E=-1.059034 Ha, Error=1.835 mHa
Eval 222: E=-1.059050 Ha, Error=1.818 mHa
Eval 223: E=-1.059026 Ha, Error=1.842 mHa
Eval 224: E=-1.059050 Ha, Error=1.818 mHa
Eval 225: E=-1.059049 Ha, Error=1.819 mHa
Eval 226: E=-1.059049 Ha, Error=1.819 mHa
Eval 227: E=-1.059025 Ha, Error=1.843 mHa
Eval 228: E=-1.059050 Ha, Error=1.818 mHa
Eval 229: E=-1.059016 Ha, Error=1.852 mHa
Eval 230: E=-1.059049 Ha, Error=1.819 mHa
Eval 231: E=-1.059048 Ha, Error=1.821 mHa
Eval 232: E=-1.059049 Ha, Error=1.819 mHa
Eval 233: E=-1.059016 Ha, Error=1.852 mHa
Eval 234: E=-1.059048 Ha, Error=1.820 mHa
Eval 235: E=-1.059043 Ha, Error=1.825 mHa
Eval 236: E=-1.059050 Ha, Error=1.818 mHa
Eval 237: E=-1.059016 Ha, Error=1.852 mHa
Eval 238: E=-1.059050 Ha, Error=1.818 mHa
Eval 239: E=-1.059047 Ha, Error=1.822 mHa
Eval 240: E=-1.059050 Ha, Error=1.818 mHa
Eval 241: E=-1.059017 Ha, Error=1.851 mHa
Eval 242: E=-1.059050 Ha, Error=1.818 mHa
Eval 243: E=-1.059025 Ha, Error=1.843 mHa
Eval 244: E=-1.059050 Ha, Error=1.818 mHa
Eval 245: E=-1.059050 Ha, Error=1.819 mHa

Eval 246: E=-1.059050 Ha, Error=1.818 mHa
Eval 247: E=-1.059025 Ha, Error=1.843 mHa
Eval 248: E=-1.059042 Ha, Error=1.826 mHa
Eval 249: E=-1.059050 Ha, Error=1.818 mHa
Eval 250: E=-1.059049 Ha, Error=1.819 mHa
Eval 251: E=-1.059050 Ha, Error=1.818 mHa
Eval 252: E=-1.059050 Ha, Error=1.818 mHa
Eval 253: E=-1.059050 Ha, Error=1.818 mHa
Eval 254: E=-1.059050 Ha, Error=1.818 mHa
Eval 255: E=-1.059050 Ha, Error=1.818 mHa
Eval 256: E=-1.059050 Ha, Error=1.818 mHa
Eval 257: E=-1.059050 Ha, Error=1.818 mHa
Eval 258: E=-1.059050 Ha, Error=1.818 mHa
Eval 259: E=-1.059050 Ha, Error=1.818 mHa
Eval 260: E=-1.059050 Ha, Error=1.818 mHa
Eval 261: E=-1.059050 Ha, Error=1.818 mHa
Eval 262: E=-1.059050 Ha, Error=1.818 mHa
Eval 263: E=-1.059050 Ha, Error=1.818 mHa
Eval 264: E=-1.059050 Ha, Error=1.818 mHa
Eval 265: E=-1.059050 Ha, Error=1.818 mHa
Eval 266: E=-1.059050 Ha, Error=1.818 mHa
Eval 267: E=-1.059050 Ha, Error=1.818 mHa
Eval 268: E=-1.059050 Ha, Error=1.818 mHa
Eval 269: E=-1.059050 Ha, Error=1.818 mHa
Eval 270: E=-1.059050 Ha, Error=1.818 mHa
Eval 271: E=-1.059050 Ha, Error=1.818 mHa
Eval 272: E=-1.059050 Ha, Error=1.818 mHa
Eval 273: E=-1.059050 Ha, Error=1.818 mHa
Eval 274: E=-1.059050 Ha, Error=1.818 mHa
Eval 275: E=-1.059050 Ha, Error=1.818 mHa
Eval 276: E=-1.059050 Ha, Error=1.818 mHa
Eval 277: E=-1.059050 Ha, Error=1.818 mHa
Eval 278: E=-1.059050 Ha, Error=1.818 mHa
Eval 279: E=-1.059050 Ha, Error=1.818 mHa
Eval 280: E=-1.059050 Ha, Error=1.818 mHa
Eval 281: E=-1.059050 Ha, Error=1.818 mHa
Eval 282: E=-1.059050 Ha, Error=1.818 mHa
Eval 283: E=-1.059050 Ha, Error=1.818 mHa
Eval 284: E=-1.059050 Ha, Error=1.818 mHa
Eval 285: E=-1.059050 Ha, Error=1.818 mHa
Eval 286: E=-1.059050 Ha, Error=1.818 mHa
Eval 287: E=-1.059050 Ha, Error=1.818 mHa
Eval 288: E=-1.059050 Ha, Error=1.818 mHa
Eval 289: E=-1.059050 Ha, Error=1.818 mHa
Eval 290: E=-1.059050 Ha, Error=1.818 mHa
Eval 291: E=-1.059050 Ha, Error=1.818 mHa
Eval 292: E=-1.059050 Ha, Error=1.818 mHa
Eval 293: E=-1.059050 Ha, Error=1.818 mHa

```
Eval 294: E=-1.059050 Ha, Error=1.818 mHa  
Eval 295: E=-1.059050 Ha, Error=1.818 mHa  
Eval 296: E=-1.059050 Ha, Error=1.818 mHa  
Eval 297: E=-1.059050 Ha, Error=1.818 mHa  
Eval 298: E=-1.059050 Ha, Error=1.818 mHa  
Eval 299: E=-1.059050 Ha, Error=1.818 mHa  
Eval 300: E=-1.059050 Ha, Error=1.818 mHa  
VQE compute_minimum_eigenvalue took: 176.1s
```

```
Completed in 176.1s  
Function evaluations: 300  
Callback captured: 300 points  
Energy Error: 1.817863e-03 Ha (0.1714%)  
Fidelity: 0.997039  
Convergence: 300/300 iterations
```

```
Progress: 4/15 complete  
Elapsed: 6.6 min | Estimated remaining: 18.1 min
```

```
#####
BENCHMARK 5/15  
Ansatz: UpCCGSD | Run: 2/3  
#####
```

```
=====  
Running: UpCCGSD - Run #2  
Optimizer: COBYLA (maxiter=300)  
Parameters: 36, Depth: 37  
=====
```

```
Starting VQE optimization now...  
Eval 1: E=-1.058978 Ha, Error=1.890 mHa  
Eval 2: E=-0.914874 Ha, Error=145.995 mHa  
Eval 3: E=-1.058978 Ha, Error=1.890 mHa  
Eval 4: E=-1.058978 Ha, Error=1.890 mHa  
Eval 5: E=-1.058981 Ha, Error=1.887 mHa  
Eval 6: E=-1.058981 Ha, Error=1.887 mHa  
Eval 7: E=-1.058981 Ha, Error=1.887 mHa  
Eval 8: E=-0.929949 Ha, Error=130.919 mHa  
Eval 9: E=-1.058981 Ha, Error=1.887 mHa  
Eval 10: E=-1.058981 Ha, Error=1.887 mHa  
Eval 11: E=-0.931872 Ha, Error=128.996 mHa  
Eval 12: E=-1.058981 Ha, Error=1.887 mHa  
Eval 13: E=-1.058981 Ha, Error=1.887 mHa  
Eval 14: E=-1.058894 Ha, Error=1.974 mHa  
Eval 15: E=-1.058981 Ha, Error=1.887 mHa  
Eval 16: E=-1.058981 Ha, Error=1.887 mHa  
Eval 17: E=-0.913208 Ha, Error=147.660 mHa
```

Eval 18: E=-1.058981 Ha, Error=1.887 mHa
Eval 19: E=-1.058981 Ha, Error=1.887 mHa
Eval 20: E=-0.914278 Ha, Error=146.590 mHa
Eval 21: E=-1.058981 Ha, Error=1.887 mHa
Eval 22: E=-1.058981 Ha, Error=1.887 mHa
Eval 23: E=-1.059029 Ha, Error=1.839 mHa
Eval 24: E=-1.059029 Ha, Error=1.839 mHa
Eval 25: E=-1.059029 Ha, Error=1.839 mHa
Eval 26: E=-0.930757 Ha, Error=130.111 mHa
Eval 27: E=-1.059029 Ha, Error=1.839 mHa
Eval 28: E=-1.059029 Ha, Error=1.839 mHa
Eval 29: E=-0.931442 Ha, Error=129.426 mHa
Eval 30: E=-1.059029 Ha, Error=1.839 mHa
Eval 31: E=-1.059029 Ha, Error=1.839 mHa
Eval 32: E=-1.058997 Ha, Error=1.871 mHa
Eval 33: E=-1.059029 Ha, Error=1.839 mHa
Eval 34: E=-1.059029 Ha, Error=1.839 mHa
Eval 35: E=-0.916426 Ha, Error=144.442 mHa
Eval 36: E=-1.059029 Ha, Error=1.839 mHa
Eval 37: E=-1.059029 Ha, Error=1.839 mHa
Eval 38: E=-0.770598 Ha, Error=290.270 mHa
Eval 39: E=-1.054813 Ha, Error=6.055 mHa
Eval 40: E=-1.059029 Ha, Error=1.839 mHa
Eval 41: E=-1.051067 Ha, Error=9.801 mHa
Eval 42: E=-1.059029 Ha, Error=1.839 mHa
Eval 43: E=-1.055260 Ha, Error=5.608 mHa
Eval 44: E=-1.059011 Ha, Error=1.857 mHa
Eval 45: E=-1.057839 Ha, Error=3.029 mHa
Eval 46: E=-1.059017 Ha, Error=1.851 mHa
Eval 47: E=-1.057670 Ha, Error=3.198 mHa
Eval 48: E=-1.059013 Ha, Error=1.855 mHa
Eval 49: E=-1.056760 Ha, Error=4.108 mHa
Eval 50: E=-1.059029 Ha, Error=1.839 mHa
Eval 51: E=-1.057550 Ha, Error=3.318 mHa
Eval 52: E=-1.059029 Ha, Error=1.839 mHa
Eval 53: E=-1.057242 Ha, Error=3.626 mHa
Eval 54: E=-1.059030 Ha, Error=1.839 mHa
Eval 55: E=-1.057186 Ha, Error=3.682 mHa
Eval 56: E=-1.059030 Ha, Error=1.838 mHa
Eval 57: E=-1.057552 Ha, Error=3.316 mHa
Eval 58: E=-1.059032 Ha, Error=1.836 mHa
Eval 59: E=-1.058814 Ha, Error=2.054 mHa
Eval 60: E=-1.059032 Ha, Error=1.837 mHa
Eval 61: E=-1.056883 Ha, Error=3.985 mHa
Eval 62: E=-1.059032 Ha, Error=1.836 mHa
Eval 63: E=-1.056265 Ha, Error=4.603 mHa
Eval 64: E=-1.059032 Ha, Error=1.837 mHa
Eval 65: E=-1.056701 Ha, Error=4.167 mHa

Eval 66: E=-1.059032 Ha, Error=1.837 mHa
Eval 67: E=-1.058808 Ha, Error=2.060 mHa
Eval 68: E=-1.059032 Ha, Error=1.836 mHa
Eval 69: E=-1.057115 Ha, Error=3.753 mHa
Eval 70: E=-1.059031 Ha, Error=1.837 mHa
Eval 71: E=-1.057411 Ha, Error=3.457 mHa
Eval 72: E=-1.059031 Ha, Error=1.837 mHa
Eval 73: E=-1.057128 Ha, Error=3.740 mHa
Eval 74: E=-1.059032 Ha, Error=1.836 mHa
Eval 75: E=-1.057536 Ha, Error=3.332 mHa
Eval 76: E=-1.059032 Ha, Error=1.836 mHa
Eval 77: E=-1.058928 Ha, Error=1.940 mHa
Eval 78: E=-1.059032 Ha, Error=1.836 mHa
Eval 79: E=-1.057865 Ha, Error=3.004 mHa
Eval 80: E=-1.059032 Ha, Error=1.836 mHa
Eval 81: E=-1.056951 Ha, Error=3.917 mHa
Eval 82: E=-1.059032 Ha, Error=1.836 mHa
Eval 83: E=-1.056428 Ha, Error=4.440 mHa
Eval 84: E=-1.059032 Ha, Error=1.836 mHa
Eval 85: E=-1.056618 Ha, Error=4.250 mHa
Eval 86: E=-1.059032 Ha, Error=1.836 mHa
Eval 87: E=-1.057556 Ha, Error=3.312 mHa
Eval 88: E=-1.059032 Ha, Error=1.836 mHa
Eval 89: E=-1.057151 Ha, Error=3.717 mHa
Eval 90: E=-1.059032 Ha, Error=1.836 mHa
Eval 91: E=-1.057084 Ha, Error=3.784 mHa
Eval 92: E=-1.059033 Ha, Error=1.836 mHa
Eval 93: E=-1.058884 Ha, Error=1.984 mHa
Eval 94: E=-1.059032 Ha, Error=1.836 mHa
Eval 95: E=-1.058883 Ha, Error=1.985 mHa
Eval 96: E=-1.058624 Ha, Error=2.244 mHa
Eval 97: E=-1.059030 Ha, Error=1.838 mHa
Eval 98: E=-1.058942 Ha, Error=1.926 mHa
Eval 99: E=-1.059034 Ha, Error=1.834 mHa
Eval 100: E=-1.059036 Ha, Error=1.832 mHa
Eval 101: E=-1.059032 Ha, Error=1.836 mHa
Eval 102: E=-1.059035 Ha, Error=1.833 mHa
Eval 103: E=-1.058978 Ha, Error=1.890 mHa
Eval 104: E=-1.059036 Ha, Error=1.832 mHa
Eval 105: E=-1.059014 Ha, Error=1.854 mHa
Eval 106: E=-1.059038 Ha, Error=1.830 mHa
Eval 107: E=-1.059016 Ha, Error=1.853 mHa
Eval 108: E=-1.059038 Ha, Error=1.830 mHa
Eval 109: E=-1.059046 Ha, Error=1.823 mHa
Eval 110: E=-1.059036 Ha, Error=1.832 mHa
Eval 111: E=-1.059046 Ha, Error=1.823 mHa
Eval 112: E=-1.059046 Ha, Error=1.823 mHa
Eval 113: E=-1.059046 Ha, Error=1.823 mHa

Eval 114: E=-1.059040 Ha, Error=1.828 mHa
Eval 115: E=-1.059046 Ha, Error=1.822 mHa
Eval 116: E=-1.059047 Ha, Error=1.822 mHa
Eval 117: E=-1.059017 Ha, Error=1.851 mHa
Eval 118: E=-1.059047 Ha, Error=1.822 mHa
Eval 119: E=-1.059027 Ha, Error=1.841 mHa
Eval 120: E=-1.059047 Ha, Error=1.821 mHa
Eval 121: E=-1.059049 Ha, Error=1.819 mHa
Eval 122: E=-1.059048 Ha, Error=1.820 mHa
Eval 123: E=-1.059049 Ha, Error=1.819 mHa
Eval 124: E=-1.059048 Ha, Error=1.820 mHa
Eval 125: E=-1.059049 Ha, Error=1.819 mHa
Eval 126: E=-1.059041 Ha, Error=1.827 mHa
Eval 127: E=-1.059049 Ha, Error=1.819 mHa
Eval 128: E=-1.059034 Ha, Error=1.834 mHa
Eval 129: E=-1.059049 Ha, Error=1.819 mHa
Eval 130: E=-1.059023 Ha, Error=1.846 mHa
Eval 131: E=-1.059049 Ha, Error=1.819 mHa
Eval 132: E=-1.059049 Ha, Error=1.819 mHa
Eval 133: E=-1.059036 Ha, Error=1.832 mHa
Eval 134: E=-1.059049 Ha, Error=1.819 mHa
Eval 135: E=-1.059047 Ha, Error=1.821 mHa
Eval 136: E=-1.059049 Ha, Error=1.819 mHa
Eval 137: E=-1.059045 Ha, Error=1.824 mHa
Eval 138: E=-1.059049 Ha, Error=1.819 mHa
Eval 139: E=-1.059045 Ha, Error=1.823 mHa
Eval 140: E=-1.059049 Ha, Error=1.819 mHa
Eval 141: E=-1.059048 Ha, Error=1.820 mHa
Eval 142: E=-1.059049 Ha, Error=1.819 mHa
Eval 143: E=-1.059030 Ha, Error=1.838 mHa
Eval 144: E=-1.059049 Ha, Error=1.819 mHa
Eval 145: E=-1.059025 Ha, Error=1.843 mHa
Eval 146: E=-1.059049 Ha, Error=1.819 mHa
Eval 147: E=-1.059046 Ha, Error=1.822 mHa
Eval 148: E=-1.059049 Ha, Error=1.819 mHa
Eval 149: E=-1.059043 Ha, Error=1.825 mHa
Eval 150: E=-1.059049 Ha, Error=1.819 mHa
Eval 151: E=-1.059037 Ha, Error=1.831 mHa
Eval 152: E=-1.059043 Ha, Error=1.825 mHa
Eval 153: E=-1.059024 Ha, Error=1.844 mHa
Eval 154: E=-1.059039 Ha, Error=1.829 mHa
Eval 155: E=-1.059043 Ha, Error=1.825 mHa
Eval 156: E=-1.059049 Ha, Error=1.819 mHa
Eval 157: E=-1.059046 Ha, Error=1.823 mHa
Eval 158: E=-1.059050 Ha, Error=1.819 mHa
Eval 159: E=-1.059045 Ha, Error=1.823 mHa
Eval 160: E=-1.059046 Ha, Error=1.822 mHa
Eval 161: E=-1.059049 Ha, Error=1.819 mHa

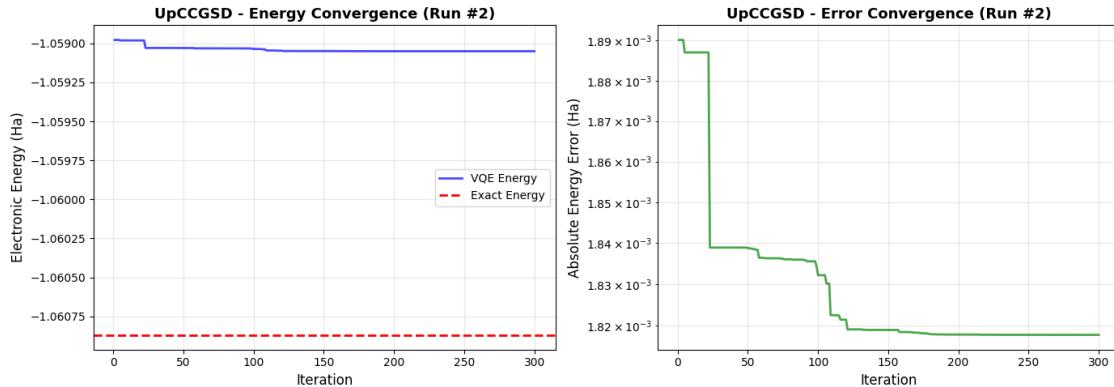
Eval 162: E=-1.059050 Ha, Error=1.819 mHa
Eval 163: E=-1.059036 Ha, Error=1.832 mHa
Eval 164: E=-1.059050 Ha, Error=1.819 mHa
Eval 165: E=-1.059043 Ha, Error=1.826 mHa
Eval 166: E=-1.059042 Ha, Error=1.826 mHa
Eval 167: E=-1.059050 Ha, Error=1.818 mHa
Eval 168: E=-1.059050 Ha, Error=1.818 mHa
Eval 169: E=-1.059050 Ha, Error=1.818 mHa
Eval 170: E=-1.059049 Ha, Error=1.819 mHa
Eval 171: E=-1.059050 Ha, Error=1.818 mHa
Eval 172: E=-1.059050 Ha, Error=1.818 mHa
Eval 173: E=-1.059050 Ha, Error=1.818 mHa
Eval 174: E=-1.059050 Ha, Error=1.818 mHa
Eval 175: E=-1.059050 Ha, Error=1.818 mHa
Eval 176: E=-1.059050 Ha, Error=1.818 mHa
Eval 177: E=-1.059049 Ha, Error=1.819 mHa
Eval 178: E=-1.059050 Ha, Error=1.818 mHa
Eval 179: E=-1.059050 Ha, Error=1.818 mHa
Eval 180: E=-1.059050 Ha, Error=1.818 mHa
Eval 181: E=-1.059050 Ha, Error=1.818 mHa
Eval 182: E=-1.059050 Ha, Error=1.818 mHa
Eval 183: E=-1.059050 Ha, Error=1.818 mHa
Eval 184: E=-1.059050 Ha, Error=1.818 mHa
Eval 185: E=-1.059050 Ha, Error=1.818 mHa
Eval 186: E=-1.059050 Ha, Error=1.818 mHa
Eval 187: E=-1.059050 Ha, Error=1.818 mHa
Eval 188: E=-1.059050 Ha, Error=1.818 mHa
Eval 189: E=-1.059050 Ha, Error=1.818 mHa
Eval 190: E=-1.059050 Ha, Error=1.818 mHa
Eval 191: E=-1.059050 Ha, Error=1.818 mHa
Eval 192: E=-1.059050 Ha, Error=1.818 mHa
Eval 193: E=-1.059050 Ha, Error=1.818 mHa
Eval 194: E=-1.059050 Ha, Error=1.818 mHa
Eval 195: E=-1.059050 Ha, Error=1.818 mHa
Eval 196: E=-1.059050 Ha, Error=1.818 mHa
Eval 197: E=-1.059050 Ha, Error=1.818 mHa
Eval 198: E=-1.059050 Ha, Error=1.818 mHa
Eval 199: E=-1.059050 Ha, Error=1.818 mHa
Eval 200: E=-1.059050 Ha, Error=1.818 mHa
Eval 201: E=-1.059050 Ha, Error=1.818 mHa
Eval 202: E=-1.059050 Ha, Error=1.818 mHa
Eval 203: E=-1.059050 Ha, Error=1.818 mHa
Eval 204: E=-1.059050 Ha, Error=1.818 mHa
Eval 205: E=-1.059050 Ha, Error=1.818 mHa
Eval 206: E=-1.059050 Ha, Error=1.818 mHa
Eval 207: E=-1.059050 Ha, Error=1.818 mHa
Eval 208: E=-1.059050 Ha, Error=1.818 mHa
Eval 209: E=-1.059050 Ha, Error=1.818 mHa


```
Eval 258: E=-1.059050 Ha, Error=1.818 mHa
Eval 259: E=-1.059050 Ha, Error=1.818 mHa
Eval 260: E=-1.059050 Ha, Error=1.818 mHa
Eval 261: E=-1.059050 Ha, Error=1.818 mHa
Eval 262: E=-1.059050 Ha, Error=1.818 mHa
Eval 263: E=-1.059050 Ha, Error=1.818 mHa
Eval 264: E=-1.059050 Ha, Error=1.818 mHa
Eval 265: E=-1.059050 Ha, Error=1.818 mHa
Eval 266: E=-1.059050 Ha, Error=1.818 mHa
Eval 267: E=-1.059050 Ha, Error=1.818 mHa
Eval 268: E=-1.059050 Ha, Error=1.818 mHa
Eval 269: E=-1.059050 Ha, Error=1.818 mHa
Eval 270: E=-1.059050 Ha, Error=1.818 mHa
Eval 271: E=-1.059050 Ha, Error=1.818 mHa
Eval 272: E=-1.059050 Ha, Error=1.818 mHa
Eval 273: E=-1.059050 Ha, Error=1.818 mHa
Eval 274: E=-1.059050 Ha, Error=1.818 mHa
Eval 275: E=-1.059050 Ha, Error=1.818 mHa
Eval 276: E=-1.059050 Ha, Error=1.818 mHa
Eval 277: E=-1.059050 Ha, Error=1.818 mHa
Eval 278: E=-1.059050 Ha, Error=1.818 mHa
Eval 279: E=-1.059050 Ha, Error=1.818 mHa
Eval 280: E=-1.059050 Ha, Error=1.818 mHa
Eval 281: E=-1.059050 Ha, Error=1.818 mHa
Eval 282: E=-1.059050 Ha, Error=1.818 mHa
Eval 283: E=-1.059050 Ha, Error=1.818 mHa
Eval 284: E=-1.059050 Ha, Error=1.818 mHa
Eval 285: E=-1.059050 Ha, Error=1.818 mHa
Eval 286: E=-1.059050 Ha, Error=1.818 mHa
Eval 287: E=-1.059050 Ha, Error=1.818 mHa
Eval 288: E=-1.059050 Ha, Error=1.818 mHa
Eval 289: E=-1.059050 Ha, Error=1.818 mHa
Eval 290: E=-1.059050 Ha, Error=1.818 mHa
Eval 291: E=-1.059050 Ha, Error=1.818 mHa
Eval 292: E=-1.059050 Ha, Error=1.818 mHa
Eval 293: E=-1.059050 Ha, Error=1.818 mHa
Eval 294: E=-1.059050 Ha, Error=1.818 mHa
Eval 295: E=-1.059050 Ha, Error=1.818 mHa
Eval 296: E=-1.059050 Ha, Error=1.818 mHa
Eval 297: E=-1.059050 Ha, Error=1.818 mHa
Eval 298: E=-1.059050 Ha, Error=1.818 mHa
Eval 299: E=-1.059050 Ha, Error=1.818 mHa
Eval 300: E=-1.059050 Ha, Error=1.818 mHa
VQE compute_minimum_eigenvalue took: 177.1s
```

```
Completed in 177.1s
Function evaluations: 300
Callback captured: 300 points
```

Energy Error: 1.817835e-03 Ha (0.1714%)
 Fidelity: 0.997039
 Convergence: 300/300 iterations

PLOTTING CONVERGENCE FOR UpCCGSD - RUN #2



Convergence plot saved: convergence_UpCCGSD_run2.png

Progress: 5/15 complete

Elapsed: 9.6 min | Estimated remaining: 19.1 min

#####

BENCHMARK 6/15

Ansatz: UpCCGSD | Run: 3/3

#####

=====

Running: UpCCGSD - Run #3

Optimizer: COBYLA (maxiter=300)

Parameters: 36, Depth: 37

=====

Starting VQE optimization now...

```

Eval 1: E=-1.058979 Ha, Error=1.889 mHa
Eval 2: E=-0.915476 Ha, Error=145.392 mHa
Eval 3: E=-1.058979 Ha, Error=1.889 mHa
Eval 4: E=-1.058979 Ha, Error=1.889 mHa
Eval 5: E=-1.058978 Ha, Error=1.891 mHa
Eval 6: E=-1.058979 Ha, Error=1.889 mHa
Eval 7: E=-1.058979 Ha, Error=1.889 mHa
  
```

Eval 8: E=-0.933728 Ha, Error=127.140 mHa
Eval 9: E=-1.058979 Ha, Error=1.889 mHa
Eval 10: E=-1.058979 Ha, Error=1.889 mHa
Eval 11: E=-0.929771 Ha, Error=131.098 mHa
Eval 12: E=-1.058979 Ha, Error=1.889 mHa
Eval 13: E=-1.058979 Ha, Error=1.889 mHa
Eval 14: E=-1.058956 Ha, Error=1.912 mHa
Eval 15: E=-1.058979 Ha, Error=1.889 mHa
Eval 16: E=-1.058979 Ha, Error=1.889 mHa
Eval 17: E=-0.914430 Ha, Error=146.439 mHa
Eval 18: E=-1.058979 Ha, Error=1.889 mHa
Eval 19: E=-1.058979 Ha, Error=1.889 mHa
Eval 20: E=-0.915450 Ha, Error=145.418 mHa
Eval 21: E=-1.058979 Ha, Error=1.889 mHa
Eval 22: E=-1.058979 Ha, Error=1.889 mHa
Eval 23: E=-1.058963 Ha, Error=1.905 mHa
Eval 24: E=-1.058979 Ha, Error=1.889 mHa
Eval 25: E=-1.058979 Ha, Error=1.889 mHa
Eval 26: E=-0.933747 Ha, Error=127.121 mHa
Eval 27: E=-1.058979 Ha, Error=1.889 mHa
Eval 28: E=-1.058979 Ha, Error=1.889 mHa
Eval 29: E=-0.929759 Ha, Error=131.109 mHa
Eval 30: E=-1.058979 Ha, Error=1.889 mHa
Eval 31: E=-1.058979 Ha, Error=1.889 mHa
Eval 32: E=-1.058919 Ha, Error=1.950 mHa
Eval 33: E=-1.058979 Ha, Error=1.889 mHa
Eval 34: E=-1.058979 Ha, Error=1.889 mHa
Eval 35: E=-0.914463 Ha, Error=146.405 mHa
Eval 36: E=-1.058979 Ha, Error=1.889 mHa
Eval 37: E=-1.058979 Ha, Error=1.889 mHa
Eval 38: E=-0.643771 Ha, Error=417.097 mHa
Eval 39: E=-1.018698 Ha, Error=42.170 mHa
Eval 40: E=-1.031215 Ha, Error=29.653 mHa
Eval 41: E=-1.058509 Ha, Error=2.359 mHa
Eval 42: E=-1.057104 Ha, Error=3.764 mHa
Eval 43: E=-1.058979 Ha, Error=1.889 mHa
Eval 44: E=-1.056669 Ha, Error=4.199 mHa
Eval 45: E=-1.058979 Ha, Error=1.889 mHa
Eval 46: E=-1.057307 Ha, Error=3.561 mHa
Eval 47: E=-1.058979 Ha, Error=1.889 mHa
Eval 48: E=-1.056402 Ha, Error=4.466 mHa
Eval 49: E=-1.058979 Ha, Error=1.889 mHa
Eval 50: E=-1.058349 Ha, Error=2.519 mHa
Eval 51: E=-1.058979 Ha, Error=1.889 mHa
Eval 52: E=-1.056764 Ha, Error=4.104 mHa
Eval 53: E=-1.058979 Ha, Error=1.889 mHa
Eval 54: E=-1.056638 Ha, Error=4.231 mHa
Eval 55: E=-1.058979 Ha, Error=1.889 mHa

Eval 56: E=-1.055175 Ha, Error=5.693 mHa
Eval 57: E=-1.058979 Ha, Error=1.889 mHa
Eval 58: E=-1.058516 Ha, Error=2.352 mHa
Eval 59: E=-1.058982 Ha, Error=1.887 mHa
Eval 60: E=-1.055123 Ha, Error=5.745 mHa
Eval 61: E=-1.058980 Ha, Error=1.888 mHa
Eval 62: E=-1.058685 Ha, Error=2.183 mHa
Eval 63: E=-1.058985 Ha, Error=1.883 mHa
Eval 64: E=-1.055155 Ha, Error=5.713 mHa
Eval 65: E=-1.058984 Ha, Error=1.884 mHa
Eval 66: E=-1.057048 Ha, Error=3.820 mHa
Eval 67: E=-1.058987 Ha, Error=1.881 mHa
Eval 68: E=-1.055031 Ha, Error=5.837 mHa
Eval 69: E=-1.058983 Ha, Error=1.885 mHa
Eval 70: E=-1.056598 Ha, Error=4.270 mHa
Eval 71: E=-1.058990 Ha, Error=1.878 mHa
Eval 72: E=-1.056919 Ha, Error=3.949 mHa
Eval 73: E=-1.058991 Ha, Error=1.877 mHa
Eval 74: E=-1.058729 Ha, Error=2.139 mHa
Eval 75: E=-1.058994 Ha, Error=1.874 mHa
Eval 76: E=-1.056859 Ha, Error=4.009 mHa
Eval 77: E=-1.058997 Ha, Error=1.871 mHa
Eval 78: E=-1.055252 Ha, Error=5.616 mHa
Eval 79: E=-1.058999 Ha, Error=1.869 mHa
Eval 80: E=-1.057295 Ha, Error=3.574 mHa
Eval 81: E=-1.058996 Ha, Error=1.872 mHa
Eval 82: E=-1.057415 Ha, Error=3.453 mHa
Eval 83: E=-1.058999 Ha, Error=1.869 mHa
Eval 84: E=-1.057256 Ha, Error=3.612 mHa
Eval 85: E=-1.058997 Ha, Error=1.871 mHa
Eval 86: E=-1.056766 Ha, Error=4.102 mHa
Eval 87: E=-1.058999 Ha, Error=1.869 mHa
Eval 88: E=-1.056912 Ha, Error=3.956 mHa
Eval 89: E=-1.059000 Ha, Error=1.869 mHa
Eval 90: E=-1.055263 Ha, Error=5.605 mHa
Eval 91: E=-1.058999 Ha, Error=1.869 mHa
Eval 92: E=-1.058759 Ha, Error=2.110 mHa
Eval 93: E=-1.058999 Ha, Error=1.869 mHa
Eval 94: E=-1.058617 Ha, Error=2.251 mHa
Eval 95: E=-1.059000 Ha, Error=1.869 mHa
Eval 96: E=-1.057826 Ha, Error=3.042 mHa
Eval 97: E=-1.059000 Ha, Error=1.869 mHa
Eval 98: E=-1.056849 Ha, Error=4.019 mHa
Eval 99: E=-1.058962 Ha, Error=1.906 mHa
Eval 100: E=-1.059003 Ha, Error=1.865 mHa
Eval 101: E=-1.058801 Ha, Error=2.067 mHa
Eval 102: E=-1.058988 Ha, Error=1.880 mHa
Eval 103: E=-1.058943 Ha, Error=1.925 mHa

Eval 104: E=-1.059002 Ha, Error=1.866 mHa
Eval 105: E=-1.058986 Ha, Error=1.882 mHa
Eval 106: E=-1.059003 Ha, Error=1.865 mHa
Eval 107: E=-1.059007 Ha, Error=1.861 mHa
Eval 108: E=-1.058954 Ha, Error=1.914 mHa
Eval 109: E=-1.059007 Ha, Error=1.861 mHa
Eval 110: E=-1.058991 Ha, Error=1.878 mHa
Eval 111: E=-1.059007 Ha, Error=1.861 mHa
Eval 112: E=-1.059010 Ha, Error=1.858 mHa
Eval 113: E=-1.059013 Ha, Error=1.855 mHa
Eval 114: E=-1.059017 Ha, Error=1.851 mHa
Eval 115: E=-1.059013 Ha, Error=1.856 mHa
Eval 116: E=-1.059017 Ha, Error=1.851 mHa
Eval 117: E=-1.058991 Ha, Error=1.877 mHa
Eval 118: E=-1.059017 Ha, Error=1.851 mHa
Eval 119: E=-1.059040 Ha, Error=1.828 mHa
Eval 120: E=-1.059026 Ha, Error=1.842 mHa
Eval 121: E=-1.059040 Ha, Error=1.828 mHa
Eval 122: E=-1.059034 Ha, Error=1.835 mHa
Eval 123: E=-1.059040 Ha, Error=1.828 mHa
Eval 124: E=-1.059031 Ha, Error=1.837 mHa
Eval 125: E=-1.059040 Ha, Error=1.828 mHa
Eval 126: E=-1.059042 Ha, Error=1.826 mHa
Eval 127: E=-1.059022 Ha, Error=1.846 mHa
Eval 128: E=-1.059042 Ha, Error=1.826 mHa
Eval 129: E=-1.059022 Ha, Error=1.846 mHa
Eval 130: E=-1.059042 Ha, Error=1.826 mHa
Eval 131: E=-1.059032 Ha, Error=1.836 mHa
Eval 132: E=-1.059043 Ha, Error=1.825 mHa
Eval 133: E=-1.059049 Ha, Error=1.820 mHa
Eval 134: E=-1.059044 Ha, Error=1.824 mHa
Eval 135: E=-1.059049 Ha, Error=1.819 mHa
Eval 136: E=-1.059046 Ha, Error=1.822 mHa
Eval 137: E=-1.059049 Ha, Error=1.819 mHa
Eval 138: E=-1.059045 Ha, Error=1.823 mHa
Eval 139: E=-1.059049 Ha, Error=1.820 mHa
Eval 140: E=-1.059046 Ha, Error=1.822 mHa
Eval 141: E=-1.059049 Ha, Error=1.819 mHa
Eval 142: E=-1.059044 Ha, Error=1.824 mHa
Eval 143: E=-1.059049 Ha, Error=1.819 mHa
Eval 144: E=-1.059048 Ha, Error=1.820 mHa
Eval 145: E=-1.059049 Ha, Error=1.819 mHa
Eval 146: E=-1.059033 Ha, Error=1.835 mHa
Eval 147: E=-1.059049 Ha, Error=1.819 mHa
Eval 148: E=-1.059038 Ha, Error=1.831 mHa
Eval 149: E=-1.059049 Ha, Error=1.819 mHa
Eval 150: E=-1.059049 Ha, Error=1.819 mHa
Eval 151: E=-1.059046 Ha, Error=1.822 mHa

Eval 152: E=-1.059049 Ha, Error=1.819 mHa
Eval 153: E=-1.059034 Ha, Error=1.834 mHa
Eval 154: E=-1.059049 Ha, Error=1.819 mHa
Eval 155: E=-1.059047 Ha, Error=1.821 mHa
Eval 156: E=-1.059049 Ha, Error=1.819 mHa
Eval 157: E=-1.059034 Ha, Error=1.835 mHa
Eval 158: E=-1.059048 Ha, Error=1.821 mHa
Eval 159: E=-1.059049 Ha, Error=1.819 mHa
Eval 160: E=-1.059049 Ha, Error=1.819 mHa
Eval 161: E=-1.059048 Ha, Error=1.820 mHa
Eval 162: E=-1.059047 Ha, Error=1.821 mHa
Eval 163: E=-1.059042 Ha, Error=1.827 mHa
Eval 164: E=-1.059049 Ha, Error=1.819 mHa
Eval 165: E=-1.059049 Ha, Error=1.819 mHa
Eval 166: E=-1.059047 Ha, Error=1.821 mHa
Eval 167: E=-1.059031 Ha, Error=1.837 mHa
Eval 168: E=-1.059048 Ha, Error=1.821 mHa
Eval 169: E=-1.059049 Ha, Error=1.819 mHa
Eval 170: E=-1.059042 Ha, Error=1.826 mHa
Eval 171: E=-1.059048 Ha, Error=1.820 mHa
Eval 172: E=-1.059038 Ha, Error=1.830 mHa
Eval 173: E=-1.059049 Ha, Error=1.819 mHa
Eval 174: E=-1.059026 Ha, Error=1.842 mHa
Eval 175: E=-1.059049 Ha, Error=1.819 mHa
Eval 176: E=-1.059032 Ha, Error=1.836 mHa
Eval 177: E=-1.059050 Ha, Error=1.819 mHa
Eval 178: E=-1.059045 Ha, Error=1.823 mHa
Eval 179: E=-1.059050 Ha, Error=1.818 mHa
Eval 180: E=-1.059045 Ha, Error=1.823 mHa
Eval 181: E=-1.059050 Ha, Error=1.818 mHa
Eval 182: E=-1.059048 Ha, Error=1.820 mHa
Eval 183: E=-1.059050 Ha, Error=1.818 mHa
Eval 184: E=-1.059047 Ha, Error=1.821 mHa
Eval 185: E=-1.059050 Ha, Error=1.818 mHa
Eval 186: E=-1.059029 Ha, Error=1.839 mHa
Eval 187: E=-1.059050 Ha, Error=1.818 mHa
Eval 188: E=-1.059026 Ha, Error=1.842 mHa
Eval 189: E=-1.059049 Ha, Error=1.819 mHa
Eval 190: E=-1.059034 Ha, Error=1.834 mHa
Eval 191: E=-1.059050 Ha, Error=1.819 mHa
Eval 192: E=-1.059046 Ha, Error=1.822 mHa
Eval 193: E=-1.059050 Ha, Error=1.818 mHa
Eval 194: E=-1.059037 Ha, Error=1.831 mHa
Eval 195: E=-1.059050 Ha, Error=1.818 mHa
Eval 196: E=-1.059041 Ha, Error=1.827 mHa
Eval 197: E=-1.059050 Ha, Error=1.818 mHa
Eval 198: E=-1.059026 Ha, Error=1.842 mHa
Eval 199: E=-1.059050 Ha, Error=1.818 mHa

Eval 200: E=-1.059049 Ha, Error=1.820 mHa
Eval 201: E=-1.059050 Ha, Error=1.818 mHa
Eval 202: E=-1.059025 Ha, Error=1.843 mHa
Eval 203: E=-1.059049 Ha, Error=1.819 mHa
Eval 204: E=-1.059050 Ha, Error=1.818 mHa
Eval 205: E=-1.059050 Ha, Error=1.818 mHa
Eval 206: E=-1.059024 Ha, Error=1.844 mHa
Eval 207: E=-1.059050 Ha, Error=1.818 mHa
Eval 208: E=-1.059050 Ha, Error=1.818 mHa
Eval 209: E=-1.059046 Ha, Error=1.822 mHa
Eval 210: E=-1.059050 Ha, Error=1.818 mHa
Eval 211: E=-1.059049 Ha, Error=1.819 mHa
Eval 212: E=-1.059050 Ha, Error=1.818 mHa
Eval 213: E=-1.059050 Ha, Error=1.818 mHa
Eval 214: E=-1.059050 Ha, Error=1.818 mHa
Eval 215: E=-1.059050 Ha, Error=1.818 mHa
Eval 216: E=-1.059050 Ha, Error=1.818 mHa
Eval 217: E=-1.059050 Ha, Error=1.818 mHa
Eval 218: E=-1.059050 Ha, Error=1.818 mHa
Eval 219: E=-1.059050 Ha, Error=1.818 mHa
Eval 220: E=-1.059050 Ha, Error=1.818 mHa
Eval 221: E=-1.059050 Ha, Error=1.818 mHa
Eval 222: E=-1.059050 Ha, Error=1.818 mHa
Eval 223: E=-1.059050 Ha, Error=1.818 mHa
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Eval 225: E=-1.059050 Ha, Error=1.818 mHa
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Eval 230: E=-1.059050 Ha, Error=1.818 mHa
Eval 231: E=-1.059050 Ha, Error=1.818 mHa
Eval 232: E=-1.059050 Ha, Error=1.818 mHa
Eval 233: E=-1.059050 Ha, Error=1.818 mHa
Eval 234: E=-1.059050 Ha, Error=1.818 mHa
Eval 235: E=-1.059050 Ha, Error=1.818 mHa
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Eval 237: E=-1.059050 Ha, Error=1.818 mHa
Eval 238: E=-1.059050 Ha, Error=1.818 mHa
Eval 239: E=-1.059050 Ha, Error=1.818 mHa
Eval 240: E=-1.059050 Ha, Error=1.818 mHa
Eval 241: E=-1.059050 Ha, Error=1.818 mHa
Eval 242: E=-1.059050 Ha, Error=1.818 mHa
Eval 243: E=-1.059050 Ha, Error=1.818 mHa
Eval 244: E=-1.059050 Ha, Error=1.818 mHa
Eval 245: E=-1.059050 Ha, Error=1.818 mHa
Eval 246: E=-1.059050 Ha, Error=1.818 mHa
Eval 247: E=-1.059050 Ha, Error=1.818 mHa

Eval 248: E=-1.059050 Ha, Error=1.818 mHa
Eval 249: E=-1.059050 Ha, Error=1.818 mHa
Eval 250: E=-1.059050 Ha, Error=1.818 mHa
Eval 251: E=-1.059050 Ha, Error=1.818 mHa
Eval 252: E=-1.059050 Ha, Error=1.818 mHa
Eval 253: E=-1.059050 Ha, Error=1.818 mHa
Eval 254: E=-1.059050 Ha, Error=1.818 mHa
Eval 255: E=-1.059050 Ha, Error=1.818 mHa
Eval 256: E=-1.059050 Ha, Error=1.818 mHa
Eval 257: E=-1.059050 Ha, Error=1.818 mHa
Eval 258: E=-1.059050 Ha, Error=1.818 mHa
Eval 259: E=-1.059050 Ha, Error=1.818 mHa
Eval 260: E=-1.059050 Ha, Error=1.818 mHa
Eval 261: E=-1.059050 Ha, Error=1.818 mHa
Eval 262: E=-1.059050 Ha, Error=1.818 mHa
Eval 263: E=-1.059050 Ha, Error=1.818 mHa
Eval 264: E=-1.059050 Ha, Error=1.818 mHa
Eval 265: E=-1.059050 Ha, Error=1.818 mHa
Eval 266: E=-1.059050 Ha, Error=1.818 mHa
Eval 267: E=-1.059050 Ha, Error=1.818 mHa
Eval 268: E=-1.059050 Ha, Error=1.818 mHa
Eval 269: E=-1.059050 Ha, Error=1.818 mHa
Eval 270: E=-1.059050 Ha, Error=1.818 mHa
Eval 271: E=-1.059050 Ha, Error=1.818 mHa
Eval 272: E=-1.059050 Ha, Error=1.818 mHa
Eval 273: E=-1.059050 Ha, Error=1.818 mHa
Eval 274: E=-1.059050 Ha, Error=1.818 mHa
Eval 275: E=-1.059050 Ha, Error=1.818 mHa
Eval 276: E=-1.059050 Ha, Error=1.818 mHa
Eval 277: E=-1.059050 Ha, Error=1.818 mHa
Eval 278: E=-1.059050 Ha, Error=1.818 mHa
Eval 279: E=-1.059050 Ha, Error=1.818 mHa
Eval 280: E=-1.059050 Ha, Error=1.818 mHa
Eval 281: E=-1.059050 Ha, Error=1.818 mHa
Eval 282: E=-1.059050 Ha, Error=1.818 mHa
Eval 283: E=-1.059050 Ha, Error=1.818 mHa
Eval 284: E=-1.059050 Ha, Error=1.818 mHa
Eval 285: E=-1.059050 Ha, Error=1.818 mHa
Eval 286: E=-1.059050 Ha, Error=1.818 mHa
Eval 287: E=-1.059050 Ha, Error=1.818 mHa
Eval 288: E=-1.059050 Ha, Error=1.818 mHa
Eval 289: E=-1.059050 Ha, Error=1.818 mHa
Eval 290: E=-1.059050 Ha, Error=1.818 mHa
Eval 291: E=-1.059050 Ha, Error=1.818 mHa
Eval 292: E=-1.059050 Ha, Error=1.818 mHa
Eval 293: E=-1.059050 Ha, Error=1.818 mHa
Eval 294: E=-1.059050 Ha, Error=1.818 mHa
Eval 295: E=-1.059050 Ha, Error=1.818 mHa

```
Eval 296: E=-1.059050 Ha, Error=1.818 mHa  
Eval 297: E=-1.059050 Ha, Error=1.818 mHa  
Eval 298: E=-1.059050 Ha, Error=1.818 mHa  
Eval 299: E=-1.059050 Ha, Error=1.818 mHa  
Eval 300: E=-1.059050 Ha, Error=1.818 mHa  
VQE compute_minimum_eigenvalue took: 175.6s
```

```
Completed in 175.6s  
Function evaluations: 300  
Callback captured: 300 points  
Energy Error: 1.817835e-03 Ha (0.1714%)  
Fidelity: 0.997039  
Convergence: 300/300 iterations
```

```
Progress: 6/15 complete  
Elapsed: 12.5 min | Estimated remaining: 18.7 min
```

```
#####
BENCHMARK 7/15  
Ansatz: PC-HEA | Run: 1/3  
#####
```

```
=====  
Running: PC-HEA - Run #1  
Optimizer: COBYLA (maxiter=300)  
Parameters: 96, Depth: 32  
=====
```

```
Starting VQE optimization now...  
Eval 1: E=-1.058862 Ha, Error=2.006 mHa  
Eval 2: E=-1.058862 Ha, Error=2.006 mHa  
Eval 3: E=-1.058862 Ha, Error=2.006 mHa  
Eval 4: E=-1.058862 Ha, Error=2.006 mHa  
Eval 5: E=-1.058862 Ha, Error=2.006 mHa  
Eval 6: E=-1.058862 Ha, Error=2.006 mHa  
Eval 7: E=-1.058862 Ha, Error=2.006 mHa  
Eval 8: E=-1.058862 Ha, Error=2.006 mHa  
Eval 9: E=-1.058862 Ha, Error=2.006 mHa  
Eval 10: E=-0.951842 Ha, Error=109.026 mHa  
Eval 11: E=-1.058862 Ha, Error=2.006 mHa  
Eval 12: E=-1.058811 Ha, Error=2.057 mHa  
Eval 13: E=-1.058862 Ha, Error=2.006 mHa  
Eval 14: E=-1.058862 Ha, Error=2.006 mHa  
Eval 15: E=-1.058862 Ha, Error=2.006 mHa  
Eval 16: E=-0.935407 Ha, Error=125.461 mHa  
Eval 17: E=-1.058862 Ha, Error=2.006 mHa  
Eval 18: E=-0.947128 Ha, Error=113.740 mHa  
Eval 19: E=-1.058862 Ha, Error=2.006 mHa
```

Eval 20: E=-1.058863 Ha, Error=2.005 mHa
Eval 21: E=-1.058863 Ha, Error=2.005 mHa
Eval 22: E=-1.058863 Ha, Error=2.005 mHa
Eval 23: E=-1.058863 Ha, Error=2.005 mHa
Eval 24: E=-1.058817 Ha, Error=2.051 mHa
Eval 25: E=-1.058819 Ha, Error=2.049 mHa
Eval 26: E=-1.058863 Ha, Error=2.005 mHa
Eval 27: E=-1.058842 Ha, Error=2.026 mHa
Eval 28: E=-1.058849 Ha, Error=2.019 mHa
Eval 29: E=-1.058872 Ha, Error=1.996 mHa
Eval 30: E=-1.058871 Ha, Error=1.997 mHa
Eval 31: E=-1.058872 Ha, Error=1.996 mHa
Eval 32: E=-0.951283 Ha, Error=109.585 mHa
Eval 33: E=-1.058872 Ha, Error=1.996 mHa
Eval 34: E=-1.058876 Ha, Error=1.992 mHa
Eval 35: E=-1.058876 Ha, Error=1.992 mHa
Eval 36: E=-1.058855 Ha, Error=2.013 mHa
Eval 37: E=-1.058876 Ha, Error=1.992 mHa
Eval 38: E=-0.935405 Ha, Error=125.464 mHa
Eval 39: E=-1.058876 Ha, Error=1.992 mHa
Eval 40: E=-0.948896 Ha, Error=111.972 mHa
Eval 41: E=-1.058876 Ha, Error=1.992 mHa
Eval 42: E=-1.058929 Ha, Error=1.939 mHa
Eval 43: E=-1.058929 Ha, Error=1.939 mHa
Eval 44: E=-1.058929 Ha, Error=1.939 mHa
Eval 45: E=-1.058929 Ha, Error=1.939 mHa
Eval 46: E=-1.058929 Ha, Error=1.939 mHa
Eval 47: E=-1.058929 Ha, Error=1.939 mHa
Eval 48: E=-1.058930 Ha, Error=1.938 mHa
Eval 49: E=-1.058942 Ha, Error=1.926 mHa
Eval 50: E=-1.058892 Ha, Error=1.976 mHa
Eval 51: E=-1.058932 Ha, Error=1.937 mHa
Eval 52: E=-1.058941 Ha, Error=1.927 mHa
Eval 53: E=-1.058942 Ha, Error=1.926 mHa
Eval 54: E=-0.951682 Ha, Error=109.186 mHa
Eval 55: E=-1.058942 Ha, Error=1.926 mHa
Eval 56: E=-1.058944 Ha, Error=1.924 mHa
Eval 57: E=-1.058944 Ha, Error=1.924 mHa
Eval 58: E=-1.058947 Ha, Error=1.921 mHa
Eval 59: E=-1.058947 Ha, Error=1.921 mHa
Eval 60: E=-0.933572 Ha, Error=127.296 mHa
Eval 61: E=-1.058947 Ha, Error=1.921 mHa
Eval 62: E=-0.950762 Ha, Error=110.106 mHa
Eval 63: E=-1.058947 Ha, Error=1.921 mHa
Eval 64: E=-1.058937 Ha, Error=1.931 mHa
Eval 65: E=-1.058947 Ha, Error=1.921 mHa
Eval 66: E=-1.058945 Ha, Error=1.923 mHa
Eval 67: E=-1.058947 Ha, Error=1.921 mHa

Eval 68: E=-1.058944 Ha, Error=1.924 mHa
Eval 69: E=-1.058948 Ha, Error=1.920 mHa
Eval 70: E=-1.058946 Ha, Error=1.922 mHa
Eval 71: E=-1.058942 Ha, Error=1.926 mHa
Eval 72: E=-1.058915 Ha, Error=1.953 mHa
Eval 73: E=-1.058934 Ha, Error=1.934 mHa
Eval 74: E=-1.058943 Ha, Error=1.925 mHa
Eval 75: E=-1.058948 Ha, Error=1.920 mHa
Eval 76: E=-0.950562 Ha, Error=110.306 mHa
Eval 77: E=-1.058948 Ha, Error=1.920 mHa
Eval 78: E=-1.058952 Ha, Error=1.916 mHa
Eval 79: E=-1.058952 Ha, Error=1.916 mHa
Eval 80: E=-1.058940 Ha, Error=1.928 mHa
Eval 81: E=-1.058952 Ha, Error=1.916 mHa
Eval 82: E=-0.933725 Ha, Error=127.143 mHa
Eval 83: E=-1.058952 Ha, Error=1.916 mHa
Eval 84: E=-0.951009 Ha, Error=109.859 mHa
Eval 85: E=-1.058952 Ha, Error=1.916 mHa
Eval 86: E=-1.058950 Ha, Error=1.918 mHa
Eval 87: E=-1.058952 Ha, Error=1.916 mHa
Eval 88: E=-1.058950 Ha, Error=1.918 mHa
Eval 89: E=-1.058952 Ha, Error=1.916 mHa
Eval 90: E=-1.058952 Ha, Error=1.916 mHa
Eval 91: E=-1.058952 Ha, Error=1.916 mHa
Eval 92: E=-1.058952 Ha, Error=1.916 mHa
Eval 93: E=-1.058952 Ha, Error=1.916 mHa
Eval 94: E=-1.058954 Ha, Error=1.914 mHa
Eval 95: E=-1.058954 Ha, Error=1.914 mHa
Eval 96: E=-1.058952 Ha, Error=1.916 mHa
Eval 97: E=-1.058954 Ha, Error=1.914 mHa
Eval 98: E=-0.800841 Ha, Error=260.027 mHa
Eval 99: E=-1.058954 Ha, Error=1.914 mHa
Eval 100: E=-1.027627 Ha, Error=33.241 mHa
Eval 101: E=-1.058954 Ha, Error=1.914 mHa
Eval 102: E=-1.031819 Ha, Error=29.049 mHa
Eval 103: E=-1.058954 Ha, Error=1.914 mHa
Eval 104: E=-1.018279 Ha, Error=42.589 mHa
Eval 105: E=-1.058954 Ha, Error=1.914 mHa
Eval 106: E=-0.953066 Ha, Error=107.803 mHa
Eval 107: E=-1.058954 Ha, Error=1.914 mHa
Eval 108: E=-0.914947 Ha, Error=145.921 mHa
Eval 109: E=-1.058954 Ha, Error=1.914 mHa
Eval 110: E=-0.924014 Ha, Error=136.854 mHa
Eval 111: E=-1.058953 Ha, Error=1.915 mHa
Eval 112: E=-1.020187 Ha, Error=40.682 mHa
Eval 113: E=-1.058953 Ha, Error=1.915 mHa
Eval 114: E=-0.957165 Ha, Error=103.703 mHa
Eval 115: E=-1.058953 Ha, Error=1.916 mHa

Eval 116: E=-0.941261 Ha, Error=119.607 mHa
Eval 117: E=-1.058957 Ha, Error=1.911 mHa
Eval 118: E=-0.949661 Ha, Error=111.207 mHa
Eval 119: E=-1.058959 Ha, Error=1.909 mHa
Eval 120: E=-0.920481 Ha, Error=140.387 mHa
Eval 121: E=-1.058964 Ha, Error=1.904 mHa
Eval 122: E=-1.040700 Ha, Error=20.168 mHa
Eval 123: E=-1.058966 Ha, Error=1.902 mHa
Eval 124: E=-0.920911 Ha, Error=139.957 mHa
Eval 125: E=-1.058966 Ha, Error=1.902 mHa
Eval 126: E=-0.955837 Ha, Error=105.032 mHa
Eval 127: E=-1.058957 Ha, Error=1.911 mHa
Eval 128: E=-0.970006 Ha, Error=90.862 mHa
Eval 129: E=-1.058966 Ha, Error=1.902 mHa
Eval 130: E=-1.041403 Ha, Error=19.465 mHa
Eval 131: E=-1.058954 Ha, Error=1.914 mHa
Eval 132: E=-0.944437 Ha, Error=116.431 mHa
Eval 133: E=-1.058966 Ha, Error=1.902 mHa
Eval 134: E=-0.949799 Ha, Error=111.069 mHa
Eval 135: E=-1.058974 Ha, Error=1.894 mHa
Eval 136: E=-0.786052 Ha, Error=274.816 mHa
Eval 137: E=-1.058971 Ha, Error=1.897 mHa
Eval 138: E=-1.034310 Ha, Error=26.558 mHa
Eval 139: E=-1.058969 Ha, Error=1.899 mHa
Eval 140: E=-0.920496 Ha, Error=140.372 mHa
Eval 141: E=-1.058972 Ha, Error=1.896 mHa
Eval 142: E=-0.938207 Ha, Error=122.661 mHa
Eval 143: E=-1.058957 Ha, Error=1.911 mHa
Eval 144: E=-0.927644 Ha, Error=133.224 mHa
Eval 145: E=-1.058974 Ha, Error=1.894 mHa
Eval 146: E=-0.937895 Ha, Error=122.974 mHa
Eval 147: E=-1.058967 Ha, Error=1.901 mHa
Eval 148: E=-0.953831 Ha, Error=107.038 mHa
Eval 149: E=-1.058973 Ha, Error=1.896 mHa
Eval 150: E=-0.952143 Ha, Error=108.725 mHa
Eval 151: E=-1.058971 Ha, Error=1.897 mHa
Eval 152: E=-0.957367 Ha, Error=103.502 mHa
Eval 153: E=-1.058974 Ha, Error=1.894 mHa
Eval 154: E=-0.788158 Ha, Error=272.710 mHa
Eval 155: E=-1.058972 Ha, Error=1.896 mHa
Eval 156: E=-1.043292 Ha, Error=17.576 mHa
Eval 157: E=-1.058974 Ha, Error=1.894 mHa
Eval 158: E=-0.926699 Ha, Error=134.169 mHa
Eval 159: E=-1.058974 Ha, Error=1.894 mHa
Eval 160: E=-0.791622 Ha, Error=269.246 mHa
Eval 161: E=-1.058971 Ha, Error=1.897 mHa
Eval 162: E=-1.047978 Ha, Error=12.890 mHa
Eval 163: E=-1.058974 Ha, Error=1.894 mHa

Eval 164: E=-0.794955 Ha, Error=265.914 mHa
Eval 165: E=-1.058974 Ha, Error=1.894 mHa
Eval 166: E=-0.949381 Ha, Error=111.488 mHa
Eval 167: E=-1.058974 Ha, Error=1.894 mHa
Eval 168: E=-0.796189 Ha, Error=264.679 mHa
Eval 169: E=-1.058975 Ha, Error=1.893 mHa
Eval 170: E=-0.923010 Ha, Error=137.858 mHa
Eval 171: E=-1.058970 Ha, Error=1.898 mHa
Eval 172: E=-1.056512 Ha, Error=4.356 mHa
Eval 173: E=-1.058974 Ha, Error=1.894 mHa
Eval 174: E=-0.834078 Ha, Error=226.790 mHa
Eval 175: E=-1.058982 Ha, Error=1.886 mHa
Eval 176: E=-0.923811 Ha, Error=137.057 mHa
Eval 177: E=-1.058975 Ha, Error=1.894 mHa
Eval 178: E=-1.035528 Ha, Error=25.340 mHa
Eval 179: E=-1.058976 Ha, Error=1.892 mHa
Eval 180: E=-0.858912 Ha, Error=201.956 mHa
Eval 181: E=-1.058982 Ha, Error=1.887 mHa
Eval 182: E=-0.955565 Ha, Error=105.303 mHa
Eval 183: E=-1.058982 Ha, Error=1.886 mHa
Eval 184: E=-0.954800 Ha, Error=106.068 mHa
Eval 185: E=-1.058982 Ha, Error=1.886 mHa
Eval 186: E=-1.045416 Ha, Error=15.452 mHa
Eval 187: E=-1.058981 Ha, Error=1.887 mHa
Eval 188: E=-0.931480 Ha, Error=129.389 mHa
Eval 189: E=-1.058982 Ha, Error=1.886 mHa
Eval 190: E=-0.941063 Ha, Error=119.805 mHa
Eval 191: E=-1.058982 Ha, Error=1.886 mHa
Eval 192: E=-0.924844 Ha, Error=136.025 mHa
Eval 193: E=-1.058982 Ha, Error=1.886 mHa
Eval 194: E=-1.051889 Ha, Error=8.979 mHa
Eval 195: E=-1.058982 Ha, Error=1.886 mHa
Eval 196: E=-0.843386 Ha, Error=217.482 mHa
Eval 197: E=-1.058958 Ha, Error=1.910 mHa
Eval 198: E=-0.944533 Ha, Error=116.336 mHa
Eval 199: E=-1.058982 Ha, Error=1.886 mHa
Eval 200: E=-0.962078 Ha, Error=98.790 mHa
Eval 201: E=-1.058982 Ha, Error=1.887 mHa
Eval 202: E=-0.961460 Ha, Error=99.409 mHa
Eval 203: E=-1.058982 Ha, Error=1.886 mHa
Eval 204: E=-0.970885 Ha, Error=89.983 mHa
Eval 205: E=-1.058982 Ha, Error=1.887 mHa
Eval 206: E=-0.917746 Ha, Error=143.122 mHa
Eval 207: E=-1.058982 Ha, Error=1.887 mHa
Eval 208: E=-0.947421 Ha, Error=113.447 mHa
Eval 209: E=-1.058982 Ha, Error=1.886 mHa
Eval 210: E=-0.922899 Ha, Error=137.969 mHa
Eval 211: E=-1.058982 Ha, Error=1.886 mHa

Eval 212: E=-1.040531 Ha, Error=20.337 mHa
Eval 213: E=-1.058969 Ha, Error=1.899 mHa
Eval 214: E=-0.954095 Ha, Error=106.773 mHa
Eval 215: E=-1.058976 Ha, Error=1.892 mHa
Eval 216: E=-1.017374 Ha, Error=43.494 mHa
Eval 217: E=-1.058982 Ha, Error=1.886 mHa
Eval 218: E=-0.936812 Ha, Error=124.056 mHa
Eval 219: E=-1.058982 Ha, Error=1.886 mHa
Eval 220: E=-1.017188 Ha, Error=43.680 mHa
Eval 221: E=-1.058982 Ha, Error=1.886 mHa
Eval 222: E=-0.846387 Ha, Error=214.481 mHa
Eval 223: E=-1.058983 Ha, Error=1.885 mHa
Eval 224: E=-0.942248 Ha, Error=118.620 mHa
Eval 225: E=-1.058983 Ha, Error=1.885 mHa
Eval 226: E=-1.054580 Ha, Error=6.288 mHa
Eval 227: E=-1.058983 Ha, Error=1.885 mHa
Eval 228: E=-0.851103 Ha, Error=209.765 mHa
Eval 229: E=-1.058983 Ha, Error=1.886 mHa
Eval 230: E=-0.927957 Ha, Error=132.911 mHa
Eval 231: E=-1.058983 Ha, Error=1.886 mHa
Eval 232: E=-0.957137 Ha, Error=103.731 mHa
Eval 233: E=-1.058982 Ha, Error=1.886 mHa
Eval 234: E=-0.850766 Ha, Error=210.102 mHa
Eval 235: E=-1.058982 Ha, Error=1.887 mHa
Eval 236: E=-1.026634 Ha, Error=34.234 mHa
Eval 237: E=-1.058983 Ha, Error=1.885 mHa
Eval 238: E=-0.850785 Ha, Error=210.083 mHa
Eval 239: E=-1.058983 Ha, Error=1.885 mHa
Eval 240: E=-0.918530 Ha, Error=142.338 mHa
Eval 241: E=-1.058983 Ha, Error=1.885 mHa
Eval 242: E=-0.854823 Ha, Error=206.045 mHa
Eval 243: E=-1.058983 Ha, Error=1.885 mHa
Eval 244: E=-1.050471 Ha, Error=10.397 mHa
Eval 245: E=-1.058984 Ha, Error=1.884 mHa
Eval 246: E=-1.041180 Ha, Error=19.688 mHa
Eval 247: E=-1.058984 Ha, Error=1.884 mHa
Eval 248: E=-0.918354 Ha, Error=142.515 mHa
Eval 249: E=-1.058983 Ha, Error=1.885 mHa
Eval 250: E=-0.868507 Ha, Error=192.361 mHa
Eval 251: E=-1.058984 Ha, Error=1.884 mHa
Eval 252: E=-0.932533 Ha, Error=128.335 mHa
Eval 253: E=-1.058983 Ha, Error=1.885 mHa
Eval 254: E=-1.044022 Ha, Error=16.846 mHa
Eval 255: E=-1.058984 Ha, Error=1.884 mHa
Eval 256: E=-0.942309 Ha, Error=118.559 mHa
Eval 257: E=-1.049398 Ha, Error=11.470 mHa
Eval 258: E=-0.910565 Ha, Error=150.303 mHa
Eval 259: E=-1.051369 Ha, Error=9.499 mHa

```
Eval 260: E=-0.936177 Ha, Error=124.691 mHa
Eval 261: E=-1.058985 Ha, Error=1.884 mHa
Eval 262: E=-0.948799 Ha, Error=112.069 mHa
Eval 263: E=-1.058985 Ha, Error=1.884 mHa
Eval 264: E=-1.003913 Ha, Error=56.955 mHa
Eval 265: E=-1.058984 Ha, Error=1.884 mHa
Eval 266: E=-0.957475 Ha, Error=103.393 mHa
Eval 267: E=-1.058984 Ha, Error=1.885 mHa
Eval 268: E=-0.942536 Ha, Error=118.332 mHa
Eval 269: E=-1.058984 Ha, Error=1.884 mHa
Eval 270: E=-0.969020 Ha, Error=91.849 mHa
Eval 271: E=-1.058983 Ha, Error=1.885 mHa
Eval 272: E=-0.968652 Ha, Error=92.217 mHa
Eval 273: E=-1.058983 Ha, Error=1.885 mHa
Eval 274: E=-0.877364 Ha, Error=183.504 mHa
Eval 275: E=-1.058982 Ha, Error=1.886 mHa
Eval 276: E=-0.959603 Ha, Error=101.265 mHa
Eval 277: E=-1.058978 Ha, Error=1.890 mHa
Eval 278: E=-0.973265 Ha, Error=87.603 mHa
Eval 279: E=-1.058983 Ha, Error=1.885 mHa
Eval 280: E=-0.923851 Ha, Error=137.017 mHa
Eval 281: E=-1.052053 Ha, Error=8.815 mHa
Eval 282: E=-0.882832 Ha, Error=178.036 mHa
Eval 283: E=-1.058982 Ha, Error=1.886 mHa
Eval 284: E=-0.906786 Ha, Error=154.082 mHa
Eval 285: E=-1.048926 Ha, Error=11.942 mHa
Eval 286: E=-0.894783 Ha, Error=166.085 mHa
Eval 287: E=-1.058982 Ha, Error=1.886 mHa
Eval 288: E=-0.948976 Ha, Error=111.892 mHa
Eval 289: E=-1.052518 Ha, Error=8.350 mHa
Eval 290: E=-0.901333 Ha, Error=159.535 mHa
Eval 291: E=-1.058976 Ha, Error=1.892 mHa
Eval 292: E=-0.942956 Ha, Error=117.912 mHa
Eval 293: E=-1.058983 Ha, Error=1.885 mHa
Eval 294: E=-0.900703 Ha, Error=160.165 mHa
Eval 295: E=-1.058984 Ha, Error=1.885 mHa
Eval 296: E=-0.948908 Ha, Error=111.960 mHa
Eval 297: E=-1.058982 Ha, Error=1.886 mHa
Eval 298: E=-0.900857 Ha, Error=160.011 mHa
Eval 299: E=-1.058973 Ha, Error=1.895 mHa
Eval 300: E=-0.907131 Ha, Error=153.737 mHa
VQE compute_minimum_eigenvalue took: 1.6s
```

```
Completed in 1.6s
Function evaluations: 300
Callback captured: 300 points
Energy Error: 1.883621e-03 Ha (0.1776%)
Fidelity: 0.996781
```

Convergence: 300/300 iterations

Progress: 7/15 complete

Elapsed: 12.5 min | Estimated remaining: 14.3 min

#####
BENCHMARK 8/15
Ansatz: PC-HEA | Run: 2/3
#####

=====

Running: PC-HEA - Run #2

Optimizer: COBYLA (maxiter=300)

Parameters: 96, Depth: 32

=====

Starting VQE optimization now...

Eval 1: E=-1.058849 Ha, Error=2.019 mHa
Eval 2: E=-1.058849 Ha, Error=2.019 mHa
Eval 3: E=-1.058849 Ha, Error=2.019 mHa
Eval 4: E=-1.058849 Ha, Error=2.019 mHa
Eval 5: E=-1.058849 Ha, Error=2.019 mHa
Eval 6: E=-1.058849 Ha, Error=2.019 mHa
Eval 7: E=-1.058849 Ha, Error=2.019 mHa
Eval 8: E=-1.058849 Ha, Error=2.019 mHa
Eval 9: E=-1.058849 Ha, Error=2.019 mHa
Eval 10: E=-0.950439 Ha, Error=110.429 mHa
Eval 11: E=-1.058849 Ha, Error=2.019 mHa
Eval 12: E=-1.058849 Ha, Error=2.019 mHa
Eval 13: E=-1.058849 Ha, Error=2.019 mHa
Eval 14: E=-1.058849 Ha, Error=2.019 mHa
Eval 15: E=-1.058849 Ha, Error=2.019 mHa
Eval 16: E=-0.933859 Ha, Error=127.009 mHa
Eval 17: E=-1.058849 Ha, Error=2.019 mHa
Eval 18: E=-0.945863 Ha, Error=115.005 mHa
Eval 19: E=-1.058849 Ha, Error=2.019 mHa
Eval 20: E=-1.058881 Ha, Error=1.987 mHa
Eval 21: E=-1.058881 Ha, Error=1.987 mHa
Eval 22: E=-1.058881 Ha, Error=1.987 mHa
Eval 23: E=-1.058881 Ha, Error=1.987 mHa
Eval 24: E=-1.058881 Ha, Error=1.987 mHa
Eval 25: E=-1.058881 Ha, Error=1.987 mHa
Eval 26: E=-1.058881 Ha, Error=1.987 mHa
Eval 27: E=-1.058883 Ha, Error=1.985 mHa
Eval 28: E=-1.058900 Ha, Error=1.968 mHa
Eval 29: E=-1.058881 Ha, Error=1.987 mHa
Eval 30: E=-1.058900 Ha, Error=1.968 mHa
Eval 31: E=-1.058900 Ha, Error=1.968 mHa

Eval 32: E=-0.950937 Ha, Error=109.931 mHa
Eval 33: E=-1.058900 Ha, Error=1.968 mHa
Eval 34: E=-1.058895 Ha, Error=1.974 mHa
Eval 35: E=-1.058900 Ha, Error=1.968 mHa
Eval 36: E=-1.058902 Ha, Error=1.967 mHa
Eval 37: E=-1.058902 Ha, Error=1.967 mHa
Eval 38: E=-0.933129 Ha, Error=127.739 mHa
Eval 39: E=-1.058902 Ha, Error=1.967 mHa
Eval 40: E=-0.946864 Ha, Error=114.004 mHa
Eval 41: E=-1.058902 Ha, Error=1.967 mHa
Eval 42: E=-1.058964 Ha, Error=1.904 mHa
Eval 43: E=-1.058964 Ha, Error=1.904 mHa
Eval 44: E=-1.058964 Ha, Error=1.904 mHa
Eval 45: E=-1.058964 Ha, Error=1.904 mHa
Eval 46: E=-1.058961 Ha, Error=1.907 mHa
Eval 47: E=-1.058961 Ha, Error=1.907 mHa
Eval 48: E=-1.058964 Ha, Error=1.904 mHa
Eval 49: E=-1.058957 Ha, Error=1.911 mHa
Eval 50: E=-1.058944 Ha, Error=1.924 mHa
Eval 51: E=-1.058915 Ha, Error=1.953 mHa
Eval 52: E=-1.058964 Ha, Error=1.904 mHa
Eval 53: E=-1.058964 Ha, Error=1.904 mHa
Eval 54: E=-0.950939 Ha, Error=109.929 mHa
Eval 55: E=-1.058964 Ha, Error=1.904 mHa
Eval 56: E=-1.058960 Ha, Error=1.908 mHa
Eval 57: E=-1.058964 Ha, Error=1.904 mHa
Eval 58: E=-1.058952 Ha, Error=1.916 mHa
Eval 59: E=-1.058964 Ha, Error=1.904 mHa
Eval 60: E=-0.933164 Ha, Error=127.704 mHa
Eval 61: E=-1.058964 Ha, Error=1.904 mHa
Eval 62: E=-0.947839 Ha, Error=113.029 mHa
Eval 63: E=-1.058964 Ha, Error=1.904 mHa
Eval 64: E=-1.058991 Ha, Error=1.877 mHa
Eval 65: E=-1.058991 Ha, Error=1.877 mHa
Eval 66: E=-1.058991 Ha, Error=1.877 mHa
Eval 67: E=-1.058991 Ha, Error=1.877 mHa
Eval 68: E=-1.058987 Ha, Error=1.881 mHa
Eval 69: E=-1.058987 Ha, Error=1.881 mHa
Eval 70: E=-1.058991 Ha, Error=1.877 mHa
Eval 71: E=-1.058984 Ha, Error=1.884 mHa
Eval 72: E=-1.058991 Ha, Error=1.877 mHa
Eval 73: E=-1.058984 Ha, Error=1.884 mHa
Eval 74: E=-1.058991 Ha, Error=1.877 mHa
Eval 75: E=-1.058991 Ha, Error=1.877 mHa
Eval 76: E=-0.950925 Ha, Error=109.943 mHa
Eval 77: E=-1.058991 Ha, Error=1.877 mHa
Eval 78: E=-1.058995 Ha, Error=1.873 mHa
Eval 79: E=-1.058995 Ha, Error=1.873 mHa

Eval 80: E=-1.058987 Ha, Error=1.881 mHa
Eval 81: E=-1.058995 Ha, Error=1.873 mHa
Eval 82: E=-0.932414 Ha, Error=128.454 mHa
Eval 83: E=-1.058995 Ha, Error=1.873 mHa
Eval 84: E=-0.949265 Ha, Error=111.603 mHa
Eval 85: E=-1.058995 Ha, Error=1.873 mHa
Eval 86: E=-1.058992 Ha, Error=1.877 mHa
Eval 87: E=-1.058995 Ha, Error=1.873 mHa
Eval 88: E=-1.058994 Ha, Error=1.875 mHa
Eval 89: E=-1.058995 Ha, Error=1.873 mHa
Eval 90: E=-1.058993 Ha, Error=1.875 mHa
Eval 91: E=-1.058995 Ha, Error=1.873 mHa
Eval 92: E=-1.058994 Ha, Error=1.874 mHa
Eval 93: E=-1.058995 Ha, Error=1.873 mHa
Eval 94: E=-1.058993 Ha, Error=1.875 mHa
Eval 95: E=-1.058995 Ha, Error=1.873 mHa
Eval 96: E=-1.058994 Ha, Error=1.874 mHa
Eval 97: E=-1.058995 Ha, Error=1.873 mHa
Eval 98: E=-0.684947 Ha, Error=375.921 mHa
Eval 99: E=-1.058995 Ha, Error=1.873 mHa
Eval 100: E=-1.020303 Ha, Error=40.565 mHa
Eval 101: E=-1.058995 Ha, Error=1.873 mHa
Eval 102: E=-1.033806 Ha, Error=27.062 mHa
Eval 103: E=-1.058995 Ha, Error=1.873 mHa
Eval 104: E=-0.919669 Ha, Error=141.199 mHa
Eval 105: E=-1.058995 Ha, Error=1.873 mHa
Eval 106: E=-0.963791 Ha, Error=97.078 mHa
Eval 107: E=-1.058995 Ha, Error=1.873 mHa
Eval 108: E=-0.952675 Ha, Error=108.193 mHa
Eval 109: E=-1.058995 Ha, Error=1.873 mHa
Eval 110: E=-0.941756 Ha, Error=119.112 mHa
Eval 111: E=-1.058995 Ha, Error=1.873 mHa
Eval 112: E=-0.939507 Ha, Error=121.361 mHa
Eval 113: E=-1.058995 Ha, Error=1.873 mHa
Eval 114: E=-0.923088 Ha, Error=137.780 mHa
Eval 115: E=-1.058995 Ha, Error=1.873 mHa
Eval 116: E=-0.935996 Ha, Error=124.873 mHa
Eval 117: E=-1.058995 Ha, Error=1.873 mHa
Eval 118: E=-0.927419 Ha, Error=133.449 mHa
Eval 119: E=-1.058995 Ha, Error=1.873 mHa
Eval 120: E=-0.947483 Ha, Error=113.386 mHa
Eval 121: E=-1.058998 Ha, Error=1.870 mHa
Eval 122: E=-0.931283 Ha, Error=129.585 mHa
Eval 123: E=-1.059001 Ha, Error=1.867 mHa
Eval 124: E=-1.038873 Ha, Error=21.995 mHa
Eval 125: E=-1.059003 Ha, Error=1.865 mHa
Eval 126: E=-0.942695 Ha, Error=118.173 mHa
Eval 127: E=-1.058997 Ha, Error=1.871 mHa

Eval 128: E=-0.948646 Ha, Error=112.223 mHa
Eval 129: E=-1.059003 Ha, Error=1.865 mHa
Eval 130: E=-0.714944 Ha, Error=345.924 mHa
Eval 131: E=-1.058993 Ha, Error=1.876 mHa
Eval 132: E=-1.037314 Ha, Error=23.554 mHa
Eval 133: E=-1.059003 Ha, Error=1.865 mHa
Eval 134: E=-1.044824 Ha, Error=16.045 mHa
Eval 135: E=-1.059003 Ha, Error=1.865 mHa
Eval 136: E=-1.039789 Ha, Error=21.079 mHa
Eval 137: E=-1.059003 Ha, Error=1.865 mHa
Eval 138: E=-1.051250 Ha, Error=9.618 mHa
Eval 139: E=-1.059003 Ha, Error=1.865 mHa
Eval 140: E=-0.740414 Ha, Error=320.454 mHa
Eval 141: E=-1.059007 Ha, Error=1.862 mHa
Eval 142: E=-0.928439 Ha, Error=132.430 mHa
Eval 143: E=-1.058986 Ha, Error=1.882 mHa
Eval 144: E=-1.048412 Ha, Error=12.456 mHa
Eval 145: E=-1.059006 Ha, Error=1.862 mHa
Eval 146: E=-0.926085 Ha, Error=134.783 mHa
Eval 147: E=-1.059005 Ha, Error=1.863 mHa
Eval 148: E=-0.931669 Ha, Error=129.199 mHa
Eval 149: E=-1.059007 Ha, Error=1.862 mHa
Eval 150: E=-0.940892 Ha, Error=119.976 mHa
Eval 151: E=-1.059007 Ha, Error=1.862 mHa
Eval 152: E=-0.936678 Ha, Error=124.190 mHa
Eval 153: E=-1.059005 Ha, Error=1.863 mHa
Eval 154: E=-0.943432 Ha, Error=117.436 mHa
Eval 155: E=-1.059007 Ha, Error=1.862 mHa
Eval 156: E=-0.922723 Ha, Error=138.145 mHa
Eval 157: E=-1.059009 Ha, Error=1.859 mHa
Eval 158: E=-0.949834 Ha, Error=111.034 mHa
Eval 159: E=-1.059009 Ha, Error=1.859 mHa
Eval 160: E=-1.044960 Ha, Error=15.908 mHa
Eval 161: E=-1.059009 Ha, Error=1.859 mHa
Eval 162: E=-0.772132 Ha, Error=288.737 mHa
Eval 163: E=-1.059009 Ha, Error=1.859 mHa
Eval 164: E=-0.963901 Ha, Error=96.968 mHa
Eval 165: E=-1.058993 Ha, Error=1.875 mHa
Eval 166: E=-0.954823 Ha, Error=106.046 mHa
Eval 167: E=-1.059009 Ha, Error=1.859 mHa
Eval 168: E=-0.943627 Ha, Error=117.241 mHa
Eval 169: E=-1.059008 Ha, Error=1.861 mHa
Eval 170: E=-0.949660 Ha, Error=111.208 mHa
Eval 171: E=-1.059009 Ha, Error=1.859 mHa
Eval 172: E=-0.773538 Ha, Error=287.330 mHa
Eval 173: E=-1.059007 Ha, Error=1.861 mHa
Eval 174: E=-0.922454 Ha, Error=138.414 mHa
Eval 175: E=-1.059008 Ha, Error=1.860 mHa

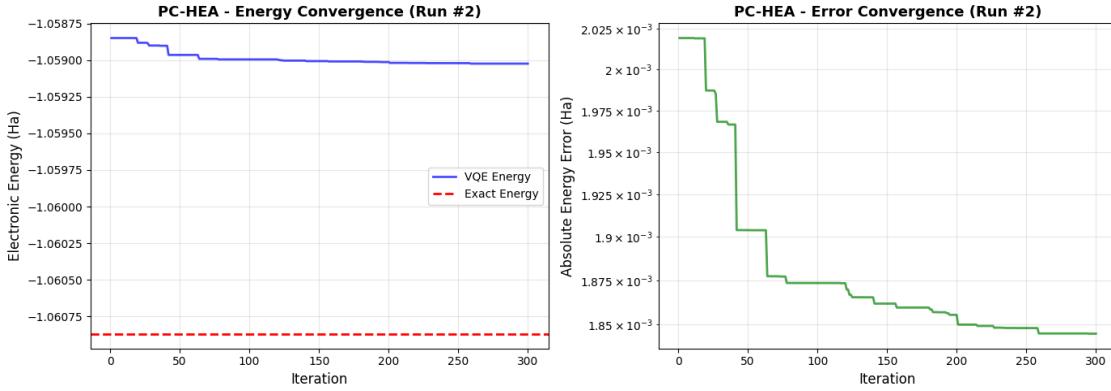
Eval 176: E=-0.778307 Ha, Error=282.562 mHa
Eval 177: E=-1.059009 Ha, Error=1.859 mHa
Eval 178: E=-0.925748 Ha, Error=135.121 mHa
Eval 179: E=-1.059005 Ha, Error=1.863 mHa
Eval 180: E=-0.779990 Ha, Error=280.879 mHa
Eval 181: E=-1.059010 Ha, Error=1.858 mHa
Eval 182: E=-0.932190 Ha, Error=128.678 mHa
Eval 183: E=-1.059011 Ha, Error=1.857 mHa
Eval 184: E=-1.050180 Ha, Error=10.688 mHa
Eval 185: E=-1.059011 Ha, Error=1.857 mHa
Eval 186: E=-0.782235 Ha, Error=278.633 mHa
Eval 187: E=-1.059011 Ha, Error=1.857 mHa
Eval 188: E=-0.932668 Ha, Error=128.200 mHa
Eval 189: E=-1.059011 Ha, Error=1.857 mHa
Eval 190: E=-0.934919 Ha, Error=125.949 mHa
Eval 191: E=-1.059008 Ha, Error=1.861 mHa
Eval 192: E=-0.942422 Ha, Error=118.446 mHa
Eval 193: E=-1.059012 Ha, Error=1.856 mHa
Eval 194: E=-0.944683 Ha, Error=116.185 mHa
Eval 195: E=-1.059013 Ha, Error=1.855 mHa
Eval 196: E=-1.033604 Ha, Error=27.264 mHa
Eval 197: E=-1.059013 Ha, Error=1.855 mHa
Eval 198: E=-0.804097 Ha, Error=256.772 mHa
Eval 199: E=-1.059013 Ha, Error=1.855 mHa
Eval 200: E=-0.950314 Ha, Error=110.554 mHa
Eval 201: E=-1.059018 Ha, Error=1.850 mHa
Eval 202: E=-0.915629 Ha, Error=145.239 mHa
Eval 203: E=-1.059018 Ha, Error=1.850 mHa
Eval 204: E=-0.931397 Ha, Error=129.471 mHa
Eval 205: E=-1.059018 Ha, Error=1.850 mHa
Eval 206: E=-0.919683 Ha, Error=141.185 mHa
Eval 207: E=-1.059018 Ha, Error=1.850 mHa
Eval 208: E=-0.948210 Ha, Error=112.659 mHa
Eval 209: E=-1.059017 Ha, Error=1.851 mHa
Eval 210: E=-0.947325 Ha, Error=113.544 mHa
Eval 211: E=-1.059018 Ha, Error=1.850 mHa
Eval 212: E=-0.956900 Ha, Error=103.968 mHa
Eval 213: E=-1.059018 Ha, Error=1.850 mHa
Eval 214: E=-0.817670 Ha, Error=243.198 mHa
Eval 215: E=-1.059019 Ha, Error=1.849 mHa
Eval 216: E=-1.044591 Ha, Error=16.277 mHa
Eval 217: E=-1.059015 Ha, Error=1.853 mHa
Eval 218: E=-0.956645 Ha, Error=104.224 mHa
Eval 219: E=-1.059017 Ha, Error=1.851 mHa
Eval 220: E=-1.044453 Ha, Error=16.415 mHa
Eval 221: E=-1.059019 Ha, Error=1.849 mHa
Eval 222: E=-0.942440 Ha, Error=118.428 mHa
Eval 223: E=-1.059019 Ha, Error=1.849 mHa

Eval 224: E=-0.932540 Ha, Error=128.328 mHa
Eval 225: E=-1.059019 Ha, Error=1.849 mHa
Eval 226: E=-1.052560 Ha, Error=8.308 mHa
Eval 227: E=-1.059020 Ha, Error=1.848 mHa
Eval 228: E=-0.940371 Ha, Error=120.497 mHa
Eval 229: E=-1.059020 Ha, Error=1.848 mHa
Eval 230: E=-0.949141 Ha, Error=111.727 mHa
Eval 231: E=-1.059018 Ha, Error=1.850 mHa
Eval 232: E=-0.827555 Ha, Error=233.314 mHa
Eval 233: E=-1.059020 Ha, Error=1.848 mHa
Eval 234: E=-1.055519 Ha, Error=5.349 mHa
Eval 235: E=-1.059020 Ha, Error=1.848 mHa
Eval 236: E=-1.044865 Ha, Error=16.003 mHa
Eval 237: E=-1.059020 Ha, Error=1.848 mHa
Eval 238: E=-0.918836 Ha, Error=142.032 mHa
Eval 239: E=-1.059020 Ha, Error=1.848 mHa
Eval 240: E=-0.922844 Ha, Error=138.024 mHa
Eval 241: E=-1.059020 Ha, Error=1.848 mHa
Eval 242: E=-0.924093 Ha, Error=136.775 mHa
Eval 243: E=-1.059020 Ha, Error=1.848 mHa
Eval 244: E=-0.827368 Ha, Error=233.500 mHa
Eval 245: E=-1.059020 Ha, Error=1.848 mHa
Eval 246: E=-1.016532 Ha, Error=44.336 mHa
Eval 247: E=-1.059020 Ha, Error=1.848 mHa
Eval 248: E=-1.028653 Ha, Error=32.215 mHa
Eval 249: E=-1.059020 Ha, Error=1.848 mHa
Eval 250: E=-1.037798 Ha, Error=23.070 mHa
Eval 251: E=-1.059020 Ha, Error=1.848 mHa
Eval 252: E=-0.954744 Ha, Error=106.124 mHa
Eval 253: E=-1.059020 Ha, Error=1.848 mHa
Eval 254: E=-0.941477 Ha, Error=119.391 mHa
Eval 255: E=-1.059020 Ha, Error=1.848 mHa
Eval 256: E=-0.947103 Ha, Error=113.765 mHa
Eval 257: E=-1.059020 Ha, Error=1.848 mHa
Eval 258: E=-0.952288 Ha, Error=108.581 mHa
Eval 259: E=-1.059023 Ha, Error=1.845 mHa
Eval 260: E=-0.940564 Ha, Error=120.304 mHa
Eval 261: E=-1.049925 Ha, Error=10.943 mHa
Eval 262: E=-1.056891 Ha, Error=3.977 mHa
Eval 263: E=-1.059023 Ha, Error=1.845 mHa
Eval 264: E=-0.935844 Ha, Error=125.024 mHa
Eval 265: E=-1.059023 Ha, Error=1.845 mHa
Eval 266: E=-0.939137 Ha, Error=121.732 mHa
Eval 267: E=-1.059023 Ha, Error=1.845 mHa
Eval 268: E=-0.963487 Ha, Error=97.381 mHa
Eval 269: E=-1.053006 Ha, Error=7.862 mHa
Eval 270: E=-0.839210 Ha, Error=221.658 mHa
Eval 271: E=-1.059023 Ha, Error=1.845 mHa

```
Eval 272: E=-0.949944 Ha, Error=110.924 mHa
Eval 273: E=-1.059023 Ha, Error=1.845 mHa
Eval 274: E=-1.056546 Ha, Error=4.322 mHa
Eval 275: E=-1.059023 Ha, Error=1.845 mHa
Eval 276: E=-0.839745 Ha, Error=221.123 mHa
Eval 277: E=-1.059023 Ha, Error=1.845 mHa
Eval 278: E=-0.927973 Ha, Error=132.895 mHa
Eval 279: E=-1.051344 Ha, Error=9.524 mHa
Eval 280: E=-0.846710 Ha, Error=214.159 mHa
Eval 281: E=-1.057056 Ha, Error=3.813 mHa
Eval 282: E=-0.920605 Ha, Error=140.264 mHa
Eval 283: E=-1.059023 Ha, Error=1.846 mHa
Eval 284: E=-0.927342 Ha, Error=133.526 mHa
Eval 285: E=-1.051204 Ha, Error=9.664 mHa
Eval 286: E=-0.862402 Ha, Error=198.466 mHa
Eval 287: E=-1.059021 Ha, Error=1.847 mHa
Eval 288: E=-0.940375 Ha, Error=120.493 mHa
Eval 289: E=-1.057477 Ha, Error=3.391 mHa
Eval 290: E=-0.866873 Ha, Error=193.995 mHa
Eval 291: E=-1.056766 Ha, Error=4.102 mHa
Eval 292: E=-0.925393 Ha, Error=135.476 mHa
Eval 293: E=-1.059023 Ha, Error=1.845 mHa
Eval 294: E=-0.866484 Ha, Error=194.384 mHa
Eval 295: E=-1.059024 Ha, Error=1.845 mHa
Eval 296: E=-0.926006 Ha, Error=134.862 mHa
Eval 297: E=-1.059021 Ha, Error=1.847 mHa
Eval 298: E=-1.051634 Ha, Error=9.234 mHa
Eval 299: E=-1.059016 Ha, Error=1.852 mHa
Eval 300: E=-0.863482 Ha, Error=197.386 mHa
VQE compute_minimum_eigenvalue took: 1.6s
```

```
Completed in 1.6s
Function evaluations: 300
Callback captured: 300 points
Energy Error: 1.844575e-03 Ha (0.1739%)
Fidelity: 0.997075
Convergence: 300/300 iterations
```

```
*****
PLOTTING CONVERGENCE FOR PC-HEA - RUN #2
*****
```



Convergence plot saved: convergence_PC-HEA_run2.png

Progress: 8/15 complete

Elapsed: 12.5 min | Estimated remaining: 11.0 min

```
#####
BENCHMARK 9/15
Ansatz: PC-HEA | Run: 3/3
#####
```

```
=====
Running: PC-HEA - Run #3
Optimizer: COBYLA (maxiter=300)
Parameters: 96, Depth: 32
=====
```

```
Starting VQE optimization now...
Eval 1: E=-1.058868 Ha, Error=2.000 mHa
Eval 2: E=-1.058868 Ha, Error=2.000 mHa
Eval 3: E=-1.058868 Ha, Error=2.000 mHa
Eval 4: E=-1.058868 Ha, Error=2.000 mHa
Eval 5: E=-1.058868 Ha, Error=2.000 mHa
Eval 6: E=-1.058868 Ha, Error=2.000 mHa
Eval 7: E=-1.058868 Ha, Error=2.000 mHa
Eval 8: E=-1.058868 Ha, Error=2.000 mHa
Eval 9: E=-1.058868 Ha, Error=2.000 mHa
Eval 10: E=-0.949727 Ha, Error=111.141 mHa
Eval 11: E=-1.058868 Ha, Error=2.000 mHa
Eval 12: E=-1.058867 Ha, Error=2.001 mHa
Eval 13: E=-1.058868 Ha, Error=2.000 mHa
Eval 14: E=-1.058868 Ha, Error=2.000 mHa
Eval 15: E=-1.058868 Ha, Error=2.000 mHa
```

Eval 16: E=-0.935921 Ha, Error=124.947 mHa
Eval 17: E=-1.058868 Ha, Error=2.000 mHa
Eval 18: E=-0.953833 Ha, Error=107.035 mHa
Eval 19: E=-1.058868 Ha, Error=2.000 mHa
Eval 20: E=-1.058884 Ha, Error=1.984 mHa
Eval 21: E=-1.058884 Ha, Error=1.984 mHa
Eval 22: E=-1.058884 Ha, Error=1.984 mHa
Eval 23: E=-1.058884 Ha, Error=1.984 mHa
Eval 24: E=-1.058884 Ha, Error=1.984 mHa
Eval 25: E=-1.058883 Ha, Error=1.985 mHa
Eval 26: E=-1.058884 Ha, Error=1.984 mHa
Eval 27: E=-1.058901 Ha, Error=1.967 mHa
Eval 28: E=-1.058895 Ha, Error=1.974 mHa
Eval 29: E=-1.058911 Ha, Error=1.957 mHa
Eval 30: E=-1.058911 Ha, Error=1.957 mHa
Eval 31: E=-1.058911 Ha, Error=1.957 mHa
Eval 32: E=-0.950214 Ha, Error=110.654 mHa
Eval 33: E=-1.058911 Ha, Error=1.957 mHa
Eval 34: E=-1.058910 Ha, Error=1.958 mHa
Eval 35: E=-1.058911 Ha, Error=1.957 mHa
Eval 36: E=-1.058919 Ha, Error=1.949 mHa
Eval 37: E=-1.058919 Ha, Error=1.949 mHa
Eval 38: E=-0.933843 Ha, Error=127.026 mHa
Eval 39: E=-1.058919 Ha, Error=1.949 mHa
Eval 40: E=-0.952824 Ha, Error=108.044 mHa
Eval 41: E=-1.058919 Ha, Error=1.949 mHa
Eval 42: E=-1.058946 Ha, Error=1.922 mHa
Eval 43: E=-1.058946 Ha, Error=1.922 mHa
Eval 44: E=-1.058946 Ha, Error=1.922 mHa
Eval 45: E=-1.058946 Ha, Error=1.922 mHa
Eval 46: E=-1.058946 Ha, Error=1.922 mHa
Eval 47: E=-1.058946 Ha, Error=1.922 mHa
Eval 48: E=-1.058946 Ha, Error=1.922 mHa
Eval 49: E=-1.058946 Ha, Error=1.922 mHa
Eval 50: E=-1.058936 Ha, Error=1.932 mHa
Eval 51: E=-1.058948 Ha, Error=1.920 mHa
Eval 52: E=-1.058948 Ha, Error=1.920 mHa
Eval 53: E=-1.058948 Ha, Error=1.920 mHa
Eval 54: E=-0.949882 Ha, Error=110.986 mHa
Eval 55: E=-1.058948 Ha, Error=1.920 mHa
Eval 56: E=-1.058937 Ha, Error=1.931 mHa
Eval 57: E=-1.058948 Ha, Error=1.920 mHa
Eval 58: E=-1.058948 Ha, Error=1.920 mHa
Eval 59: E=-1.058948 Ha, Error=1.920 mHa
Eval 60: E=-0.930948 Ha, Error=129.921 mHa
Eval 61: E=-1.058948 Ha, Error=1.920 mHa
Eval 62: E=-0.951271 Ha, Error=109.597 mHa
Eval 63: E=-1.058948 Ha, Error=1.920 mHa

Eval 64: E=-1.058973 Ha, Error=1.895 mHa
Eval 65: E=-1.058973 Ha, Error=1.895 mHa
Eval 66: E=-1.058973 Ha, Error=1.895 mHa
Eval 67: E=-1.058973 Ha, Error=1.895 mHa
Eval 68: E=-1.058963 Ha, Error=1.905 mHa
Eval 69: E=-1.058966 Ha, Error=1.902 mHa
Eval 70: E=-1.058973 Ha, Error=1.895 mHa
Eval 71: E=-1.058972 Ha, Error=1.896 mHa
Eval 72: E=-1.058969 Ha, Error=1.899 mHa
Eval 73: E=-1.058953 Ha, Error=1.915 mHa
Eval 74: E=-1.058973 Ha, Error=1.895 mHa
Eval 75: E=-1.058973 Ha, Error=1.895 mHa
Eval 76: E=-0.949735 Ha, Error=111.133 mHa
Eval 77: E=-1.058973 Ha, Error=1.895 mHa
Eval 78: E=-1.058982 Ha, Error=1.886 mHa
Eval 79: E=-1.058982 Ha, Error=1.886 mHa
Eval 80: E=-1.058982 Ha, Error=1.886 mHa
Eval 81: E=-1.058982 Ha, Error=1.886 mHa
Eval 82: E=-0.930961 Ha, Error=129.907 mHa
Eval 83: E=-1.058982 Ha, Error=1.886 mHa
Eval 84: E=-0.950203 Ha, Error=110.666 mHa
Eval 85: E=-1.058982 Ha, Error=1.886 mHa
Eval 86: E=-1.058982 Ha, Error=1.887 mHa
Eval 87: E=-1.058982 Ha, Error=1.886 mHa
Eval 88: E=-1.058982 Ha, Error=1.886 mHa
Eval 89: E=-1.058982 Ha, Error=1.886 mHa
Eval 90: E=-1.058982 Ha, Error=1.886 mHa
Eval 91: E=-1.058982 Ha, Error=1.886 mHa
Eval 92: E=-1.058982 Ha, Error=1.886 mHa
Eval 93: E=-1.058982 Ha, Error=1.886 mHa
Eval 94: E=-1.058983 Ha, Error=1.886 mHa
Eval 95: E=-1.058983 Ha, Error=1.885 mHa
Eval 96: E=-1.058982 Ha, Error=1.886 mHa
Eval 97: E=-1.058983 Ha, Error=1.885 mHa
Eval 98: E=-0.665839 Ha, Error=395.029 mHa
Eval 99: E=-1.058983 Ha, Error=1.885 mHa
Eval 100: E=-1.012117 Ha, Error=48.751 mHa
Eval 101: E=-1.058983 Ha, Error=1.885 mHa
Eval 102: E=-1.043801 Ha, Error=17.067 mHa
Eval 103: E=-1.058983 Ha, Error=1.885 mHa
Eval 104: E=-0.953050 Ha, Error=107.818 mHa
Eval 105: E=-1.058983 Ha, Error=1.885 mHa
Eval 106: E=-0.943226 Ha, Error=117.642 mHa
Eval 107: E=-1.058988 Ha, Error=1.880 mHa
Eval 108: E=-0.941965 Ha, Error=118.903 mHa
Eval 109: E=-1.058989 Ha, Error=1.880 mHa
Eval 110: E=-0.950921 Ha, Error=109.947 mHa
Eval 111: E=-1.058989 Ha, Error=1.879 mHa

Eval 112: E=-0.940836 Ha, Error=120.032 mHa
Eval 113: E=-1.058989 Ha, Error=1.879 mHa
Eval 114: E=-0.922634 Ha, Error=138.235 mHa
Eval 115: E=-1.058989 Ha, Error=1.879 mHa
Eval 116: E=-0.931744 Ha, Error=129.124 mHa
Eval 117: E=-1.058989 Ha, Error=1.879 mHa
Eval 118: E=-0.938808 Ha, Error=122.060 mHa
Eval 119: E=-1.058989 Ha, Error=1.879 mHa
Eval 120: E=-0.925345 Ha, Error=135.524 mHa
Eval 121: E=-1.058988 Ha, Error=1.880 mHa
Eval 122: E=-0.934997 Ha, Error=125.871 mHa
Eval 123: E=-1.058987 Ha, Error=1.881 mHa
Eval 124: E=-0.929424 Ha, Error=131.444 mHa
Eval 125: E=-1.058983 Ha, Error=1.885 mHa
Eval 126: E=-0.939431 Ha, Error=121.437 mHa
Eval 127: E=-1.058989 Ha, Error=1.879 mHa
Eval 128: E=-0.668943 Ha, Error=391.925 mHa
Eval 129: E=-1.058980 Ha, Error=1.888 mHa
Eval 130: E=-1.047310 Ha, Error=13.558 mHa
Eval 131: E=-1.058989 Ha, Error=1.879 mHa
Eval 132: E=-0.671430 Ha, Error=389.438 mHa
Eval 133: E=-1.058988 Ha, Error=1.880 mHa
Eval 134: E=-0.942792 Ha, Error=118.076 mHa
Eval 135: E=-1.058989 Ha, Error=1.879 mHa
Eval 136: E=-0.671688 Ha, Error=389.180 mHa
Eval 137: E=-1.058989 Ha, Error=1.879 mHa
Eval 138: E=-0.939760 Ha, Error=121.108 mHa
Eval 139: E=-1.058992 Ha, Error=1.876 mHa
Eval 140: E=-0.664679 Ha, Error=396.189 mHa
Eval 141: E=-1.058979 Ha, Error=1.889 mHa
Eval 142: E=-1.039831 Ha, Error=21.037 mHa
Eval 143: E=-1.058993 Ha, Error=1.875 mHa
Eval 144: E=-0.955712 Ha, Error=105.156 mHa
Eval 145: E=-1.058997 Ha, Error=1.871 mHa
Eval 146: E=-1.054028 Ha, Error=6.841 mHa
Eval 147: E=-1.058997 Ha, Error=1.871 mHa
Eval 148: E=-0.702555 Ha, Error=358.313 mHa
Eval 149: E=-1.058997 Ha, Error=1.871 mHa
Eval 150: E=-0.920780 Ha, Error=140.088 mHa
Eval 151: E=-1.058997 Ha, Error=1.871 mHa
Eval 152: E=-0.937729 Ha, Error=123.139 mHa
Eval 153: E=-1.058997 Ha, Error=1.871 mHa
Eval 154: E=-0.941778 Ha, Error=119.090 mHa
Eval 155: E=-1.058997 Ha, Error=1.871 mHa
Eval 156: E=-0.932553 Ha, Error=128.315 mHa
Eval 157: E=-1.058997 Ha, Error=1.871 mHa
Eval 158: E=-1.048582 Ha, Error=12.286 mHa
Eval 159: E=-1.058997 Ha, Error=1.871 mHa

Eval 160: E=-0.692076 Ha, Error=368.792 mHa
Eval 161: E=-1.058997 Ha, Error=1.871 mHa
Eval 162: E=-0.921433 Ha, Error=139.435 mHa
Eval 163: E=-1.058976 Ha, Error=1.892 mHa
Eval 164: E=-1.048875 Ha, Error=11.993 mHa
Eval 165: E=-1.058997 Ha, Error=1.871 mHa
Eval 166: E=-0.695309 Ha, Error=365.559 mHa
Eval 167: E=-1.058991 Ha, Error=1.877 mHa
Eval 168: E=-0.933051 Ha, Error=127.818 mHa
Eval 169: E=-1.058997 Ha, Error=1.871 mHa
Eval 170: E=-0.936359 Ha, Error=124.509 mHa
Eval 171: E=-1.058997 Ha, Error=1.871 mHa
Eval 172: E=-0.937824 Ha, Error=123.044 mHa
Eval 173: E=-1.058997 Ha, Error=1.871 mHa
Eval 174: E=-0.942717 Ha, Error=118.151 mHa
Eval 175: E=-1.058997 Ha, Error=1.871 mHa
Eval 176: E=-0.937659 Ha, Error=123.209 mHa
Eval 177: E=-1.058997 Ha, Error=1.871 mHa
Eval 178: E=-1.046058 Ha, Error=14.810 mHa
Eval 179: E=-1.058985 Ha, Error=1.883 mHa
Eval 180: E=-0.723257 Ha, Error=337.611 mHa
Eval 181: E=-1.058990 Ha, Error=1.878 mHa
Eval 182: E=-0.939676 Ha, Error=121.192 mHa
Eval 183: E=-1.058995 Ha, Error=1.873 mHa
Eval 184: E=-0.723311 Ha, Error=337.557 mHa
Eval 185: E=-1.058997 Ha, Error=1.871 mHa
Eval 186: E=-0.920921 Ha, Error=139.947 mHa
Eval 187: E=-1.058997 Ha, Error=1.871 mHa
Eval 188: E=-1.049971 Ha, Error=10.898 mHa
Eval 189: E=-1.058993 Ha, Error=1.876 mHa
Eval 190: E=-0.724988 Ha, Error=335.880 mHa
Eval 191: E=-1.058997 Ha, Error=1.871 mHa
Eval 192: E=-0.955031 Ha, Error=105.837 mHa
Eval 193: E=-1.058996 Ha, Error=1.872 mHa
Eval 194: E=-1.043139 Ha, Error=17.730 mHa
Eval 195: E=-1.058997 Ha, Error=1.871 mHa
Eval 196: E=-0.720676 Ha, Error=340.192 mHa
Eval 197: E=-1.058997 Ha, Error=1.871 mHa
Eval 198: E=-0.936459 Ha, Error=124.409 mHa
Eval 199: E=-1.058997 Ha, Error=1.871 mHa
Eval 200: E=-0.944764 Ha, Error=116.104 mHa
Eval 201: E=-1.058969 Ha, Error=1.899 mHa
Eval 202: E=-0.933241 Ha, Error=127.627 mHa
Eval 203: E=-1.058997 Ha, Error=1.871 mHa
Eval 204: E=-0.918089 Ha, Error=142.779 mHa
Eval 205: E=-1.058998 Ha, Error=1.870 mHa
Eval 206: E=-0.728163 Ha, Error=332.705 mHa
Eval 207: E=-1.058998 Ha, Error=1.870 mHa

Eval 208: E=-1.053955 Ha, Error=6.913 mHa
Eval 209: E=-1.058995 Ha, Error=1.873 mHa
Eval 210: E=-1.050324 Ha, Error=10.544 mHa
Eval 211: E=-1.058995 Ha, Error=1.873 mHa
Eval 212: E=-0.928697 Ha, Error=132.171 mHa
Eval 213: E=-1.058998 Ha, Error=1.870 mHa
Eval 214: E=-0.940597 Ha, Error=120.271 mHa
Eval 215: E=-1.058998 Ha, Error=1.870 mHa
Eval 216: E=-0.937732 Ha, Error=123.136 mHa
Eval 217: E=-1.058987 Ha, Error=1.882 mHa
Eval 218: E=-1.053847 Ha, Error=7.021 mHa
Eval 219: E=-1.058995 Ha, Error=1.873 mHa
Eval 220: E=-0.943943 Ha, Error=116.925 mHa
Eval 221: E=-1.058998 Ha, Error=1.870 mHa
Eval 222: E=-0.744876 Ha, Error=315.992 mHa
Eval 223: E=-1.058998 Ha, Error=1.870 mHa
Eval 224: E=-1.039936 Ha, Error=20.932 mHa
Eval 225: E=-1.058998 Ha, Error=1.870 mHa
Eval 226: E=-0.943790 Ha, Error=117.078 mHa
Eval 227: E=-1.058998 Ha, Error=1.870 mHa
Eval 228: E=-0.942440 Ha, Error=118.428 mHa
Eval 229: E=-1.058998 Ha, Error=1.870 mHa
Eval 230: E=-1.051947 Ha, Error=8.921 mHa
Eval 231: E=-1.058999 Ha, Error=1.870 mHa
Eval 232: E=-0.926319 Ha, Error=134.549 mHa
Eval 233: E=-1.058999 Ha, Error=1.870 mHa
Eval 234: E=-1.048602 Ha, Error=12.266 mHa
Eval 235: E=-1.058998 Ha, Error=1.870 mHa
Eval 236: E=-0.756148 Ha, Error=304.720 mHa
Eval 237: E=-1.058999 Ha, Error=1.870 mHa
Eval 238: E=-1.011395 Ha, Error=49.473 mHa
Eval 239: E=-1.058997 Ha, Error=1.871 mHa
Eval 240: E=-0.916924 Ha, Error=143.944 mHa
Eval 241: E=-1.058999 Ha, Error=1.870 mHa
Eval 242: E=-0.934182 Ha, Error=126.686 mHa
Eval 243: E=-1.058998 Ha, Error=1.870 mHa
Eval 244: E=-0.942576 Ha, Error=118.292 mHa
Eval 245: E=-1.058999 Ha, Error=1.870 mHa
Eval 246: E=-0.938034 Ha, Error=122.834 mHa
Eval 247: E=-1.058999 Ha, Error=1.869 mHa
Eval 248: E=-0.950603 Ha, Error=110.265 mHa
Eval 249: E=-1.058999 Ha, Error=1.869 mHa
Eval 250: E=-1.051552 Ha, Error=9.317 mHa
Eval 251: E=-1.058999 Ha, Error=1.869 mHa
Eval 252: E=-0.929193 Ha, Error=131.676 mHa
Eval 253: E=-1.058999 Ha, Error=1.869 mHa
Eval 254: E=-0.752032 Ha, Error=308.836 mHa
Eval 255: E=-1.058999 Ha, Error=1.869 mHa

```
Eval 256: E=-1.048323 Ha, Error=12.545 mHa
Eval 257: E=-1.058999 Ha, Error=1.869 mHa
Eval 258: E=-0.938567 Ha, Error=122.301 mHa
Eval 259: E=-1.058999 Ha, Error=1.869 mHa
Eval 260: E=-1.053905 Ha, Error=6.964 mHa
Eval 261: E=-1.058999 Ha, Error=1.869 mHa
Eval 262: E=-0.936101 Ha, Error=124.767 mHa
Eval 263: E=-1.053067 Ha, Error=7.801 mHa
Eval 264: E=-0.954214 Ha, Error=106.654 mHa
Eval 265: E=-1.058986 Ha, Error=1.882 mHa
Eval 266: E=-0.754755 Ha, Error=306.113 mHa
Eval 267: E=-1.058981 Ha, Error=1.887 mHa
Eval 268: E=-0.949637 Ha, Error=111.231 mHa
Eval 269: E=-1.058971 Ha, Error=1.897 mHa
Eval 270: E=-0.754670 Ha, Error=306.198 mHa
Eval 271: E=-1.058939 Ha, Error=1.929 mHa
Eval 272: E=-0.913194 Ha, Error=147.674 mHa
Eval 273: E=-1.058999 Ha, Error=1.869 mHa
Eval 274: E=-0.756941 Ha, Error=303.928 mHa
Eval 275: E=-1.055562 Ha, Error=5.306 mHa
Eval 276: E=-1.043333 Ha, Error=17.535 mHa
Eval 277: E=-1.058999 Ha, Error=1.869 mHa
Eval 278: E=-0.924529 Ha, Error=136.339 mHa
Eval 279: E=-1.054443 Ha, Error=6.426 mHa
Eval 280: E=-1.042391 Ha, Error=18.477 mHa
Eval 281: E=-1.059000 Ha, Error=1.869 mHa
Eval 282: E=-0.946468 Ha, Error=114.400 mHa
Eval 283: E=-1.058999 Ha, Error=1.869 mHa
Eval 284: E=-1.024417 Ha, Error=36.452 mHa
Eval 285: E=-1.058182 Ha, Error=2.686 mHa
Eval 286: E=-0.782686 Ha, Error=278.182 mHa
Eval 287: E=-1.058999 Ha, Error=1.869 mHa
Eval 288: E=-0.931248 Ha, Error=129.620 mHa
Eval 289: E=-1.058999 Ha, Error=1.869 mHa
Eval 290: E=-0.938726 Ha, Error=122.143 mHa
Eval 291: E=-1.058999 Ha, Error=1.869 mHa
Eval 292: E=-0.945564 Ha, Error=115.304 mHa
Eval 293: E=-1.058999 Ha, Error=1.869 mHa
Eval 294: E=-0.928707 Ha, Error=132.161 mHa
Eval 295: E=-1.058990 Ha, Error=1.879 mHa
Eval 296: E=-0.954262 Ha, Error=106.607 mHa
Eval 297: E=-1.058999 Ha, Error=1.869 mHa
Eval 298: E=-0.911400 Ha, Error=149.468 mHa
Eval 299: E=-1.058999 Ha, Error=1.869 mHa
Eval 300: E=-0.783594 Ha, Error=277.274 mHa
VQE compute_minimum_eigenvalue took: 1.6s
```

Completed in 1.6s

```
Function evaluations: 300
Callback captured: 300 points
Energy Error: 1.868644e-03 Ha (0.1761%)
Fidelity: 0.996964
Convergence: 300/300 iterations
```

```
Progress: 9/15 complete
Elapsed: 12.6 min | Estimated remaining: 8.4 min
```

```
#####
BENCHMARK 10/15
Ansatz: QEB-8q | Run: 1/3
#####
```

```
=====
Running: QEB-8q - Run #1
Optimizer: COBYLA (maxiter=300)
Parameters: 50, Depth: 149
=====
```

```
Starting VQE optimization now...
Eval 1: E=-1.059016 Ha, Error=1.853 mHa
Eval 2: E=-1.031874 Ha, Error=28.994 mHa
Eval 3: E=-1.022609 Ha, Error=38.260 mHa
Eval 4: E=-1.032442 Ha, Error=28.427 mHa
Eval 5: E=-1.031738 Ha, Error=29.130 mHa
Eval 6: E=-1.037294 Ha, Error=23.575 mHa
Eval 7: E=-1.032485 Ha, Error=28.383 mHa
Eval 8: E=-1.042575 Ha, Error=18.293 mHa
Eval 9: E=-1.047446 Ha, Error=13.422 mHa
Eval 10: E=-1.042366 Ha, Error=18.502 mHa
Eval 11: E=-1.043394 Ha, Error=17.474 mHa
Eval 12: E=-1.038061 Ha, Error=22.807 mHa
Eval 13: E=-1.043338 Ha, Error=17.530 mHa
Eval 14: E=-1.044835 Ha, Error=16.033 mHa
Eval 15: E=-1.050582 Ha, Error=10.287 mHa
Eval 16: E=-1.047507 Ha, Error=13.361 mHa
Eval 17: E=-1.048886 Ha, Error=11.982 mHa
Eval 18: E=-1.047607 Ha, Error=13.261 mHa
Eval 19: E=-1.048067 Ha, Error=12.801 mHa
Eval 20: E=-1.046781 Ha, Error=14.087 mHa
Eval 21: E=-1.048028 Ha, Error=12.840 mHa
Eval 22: E=-1.046606 Ha, Error=14.262 mHa
Eval 23: E=-1.047758 Ha, Error=13.110 mHa
Eval 24: E=-1.046460 Ha, Error=14.408 mHa
Eval 25: E=-1.046963 Ha, Error=13.905 mHa
Eval 26: E=-1.045614 Ha, Error=15.254 mHa
Eval 27: E=-1.046854 Ha, Error=14.014 mHa
```

Eval 28: E=-1.047761 Ha, Error=13.107 mHa
Eval 29: E=-1.049133 Ha, Error=11.735 mHa
Eval 30: E=-1.047845 Ha, Error=13.023 mHa
Eval 31: E=-1.048345 Ha, Error=12.523 mHa
Eval 32: E=-1.047039 Ha, Error=13.829 mHa
Eval 33: E=-1.048281 Ha, Error=12.587 mHa
Eval 34: E=-1.048529 Ha, Error=12.339 mHa
Eval 35: E=-1.049725 Ha, Error=11.143 mHa
Eval 36: E=-1.048387 Ha, Error=12.481 mHa
Eval 37: E=-1.047961 Ha, Error=12.907 mHa
Eval 38: E=-1.046620 Ha, Error=14.248 mHa
Eval 39: E=-1.048027 Ha, Error=12.841 mHa
Eval 40: E=-1.049360 Ha, Error=11.509 mHa
Eval 41: E=-1.050697 Ha, Error=10.171 mHa
Eval 42: E=-1.049425 Ha, Error=11.444 mHa
Eval 43: E=-1.048923 Ha, Error=11.945 mHa
Eval 44: E=-1.047574 Ha, Error=13.294 mHa
Eval 45: E=-1.049024 Ha, Error=11.844 mHa
Eval 46: E=-1.047802 Ha, Error=13.067 mHa
Eval 47: E=-1.049193 Ha, Error=11.675 mHa
Eval 48: E=-1.047914 Ha, Error=12.954 mHa
Eval 49: E=-1.048399 Ha, Error=12.469 mHa
Eval 50: E=-1.047097 Ha, Error=13.772 mHa
Eval 51: E=-1.048355 Ha, Error=12.513 mHa
Eval 52: E=-0.914103 Ha, Error=146.765 mHa
Eval 53: E=-1.053068 Ha, Error=7.800 mHa
Eval 54: E=-1.049669 Ha, Error=11.200 mHa
Eval 55: E=-1.058962 Ha, Error=1.906 mHa
Eval 56: E=-1.058595 Ha, Error=2.273 mHa
Eval 57: E=-1.058949 Ha, Error=1.919 mHa
Eval 58: E=-1.058910 Ha, Error=1.958 mHa
Eval 59: E=-1.059012 Ha, Error=1.856 mHa
Eval 60: E=-1.058853 Ha, Error=2.015 mHa
Eval 61: E=-1.059024 Ha, Error=1.844 mHa
Eval 62: E=-1.058821 Ha, Error=2.048 mHa
Eval 63: E=-1.059026 Ha, Error=1.842 mHa
Eval 64: E=-1.057287 Ha, Error=3.582 mHa
Eval 65: E=-1.058977 Ha, Error=1.891 mHa
Eval 66: E=-1.058874 Ha, Error=1.995 mHa
Eval 67: E=-1.058989 Ha, Error=1.879 mHa
Eval 68: E=-1.059005 Ha, Error=1.863 mHa
Eval 69: E=-1.059001 Ha, Error=1.867 mHa
Eval 70: E=-1.058974 Ha, Error=1.894 mHa
Eval 71: E=-1.059018 Ha, Error=1.851 mHa
Eval 72: E=-1.058966 Ha, Error=1.902 mHa
Eval 73: E=-1.059019 Ha, Error=1.849 mHa
Eval 74: E=-1.058993 Ha, Error=1.875 mHa
Eval 75: E=-1.058989 Ha, Error=1.879 mHa

Eval 76: E=-1.058927 Ha, Error=1.941 mHa
Eval 77: E=-1.059024 Ha, Error=1.844 mHa
Eval 78: E=-1.058868 Ha, Error=2.000 mHa
Eval 79: E=-1.059006 Ha, Error=1.862 mHa
Eval 80: E=-1.058902 Ha, Error=1.967 mHa
Eval 81: E=-1.058998 Ha, Error=1.871 mHa
Eval 82: E=-1.058979 Ha, Error=1.889 mHa
Eval 83: E=-1.059009 Ha, Error=1.859 mHa
Eval 84: E=-1.058938 Ha, Error=1.930 mHa
Eval 85: E=-1.059001 Ha, Error=1.868 mHa
Eval 86: E=-1.058983 Ha, Error=1.886 mHa
Eval 87: E=-1.058987 Ha, Error=1.881 mHa
Eval 88: E=-1.058964 Ha, Error=1.904 mHa
Eval 89: E=-1.059010 Ha, Error=1.858 mHa
Eval 90: E=-1.058978 Ha, Error=1.890 mHa
Eval 91: E=-1.059037 Ha, Error=1.832 mHa
Eval 92: E=-1.058984 Ha, Error=1.884 mHa
Eval 93: E=-1.059020 Ha, Error=1.848 mHa
Eval 94: E=-1.058962 Ha, Error=1.906 mHa
Eval 95: E=-1.059023 Ha, Error=1.845 mHa
Eval 96: E=-1.058902 Ha, Error=1.966 mHa
Eval 97: E=-1.059033 Ha, Error=1.835 mHa
Eval 98: E=-1.058938 Ha, Error=1.930 mHa
Eval 99: E=-1.059044 Ha, Error=1.824 mHa
Eval 100: E=-1.058892 Ha, Error=1.976 mHa
Eval 101: E=-1.059042 Ha, Error=1.826 mHa
Eval 102: E=-1.058891 Ha, Error=1.977 mHa
Eval 103: E=-1.059046 Ha, Error=1.823 mHa
Eval 104: E=-1.058759 Ha, Error=2.109 mHa
Eval 105: E=-1.059016 Ha, Error=1.852 mHa
Eval 106: E=-1.058107 Ha, Error=2.761 mHa
Eval 107: E=-1.058728 Ha, Error=2.140 mHa
Eval 108: E=-1.059043 Ha, Error=1.826 mHa
Eval 109: E=-1.059041 Ha, Error=1.827 mHa
Eval 110: E=-1.059047 Ha, Error=1.821 mHa
Eval 111: E=-1.059043 Ha, Error=1.825 mHa
Eval 112: E=-1.059046 Ha, Error=1.822 mHa
Eval 113: E=-1.059043 Ha, Error=1.825 mHa
Eval 114: E=-1.059047 Ha, Error=1.821 mHa
Eval 115: E=-1.059043 Ha, Error=1.825 mHa
Eval 116: E=-1.059047 Ha, Error=1.821 mHa
Eval 117: E=-1.059044 Ha, Error=1.824 mHa
Eval 118: E=-1.059045 Ha, Error=1.823 mHa
Eval 119: E=-1.059047 Ha, Error=1.821 mHa
Eval 120: E=-1.059046 Ha, Error=1.822 mHa
Eval 121: E=-1.059038 Ha, Error=1.830 mHa
Eval 122: E=-1.059046 Ha, Error=1.822 mHa
Eval 123: E=-1.059046 Ha, Error=1.822 mHa

Eval 124: E=-1.059046 Ha, Error=1.822 mHa
Eval 125: E=-1.059048 Ha, Error=1.820 mHa
Eval 126: E=-1.059047 Ha, Error=1.822 mHa
Eval 127: E=-1.059048 Ha, Error=1.820 mHa
Eval 128: E=-1.059048 Ha, Error=1.820 mHa
Eval 129: E=-1.059049 Ha, Error=1.819 mHa
Eval 130: E=-1.059050 Ha, Error=1.818 mHa
Eval 131: E=-1.059049 Ha, Error=1.819 mHa
Eval 132: E=-1.059049 Ha, Error=1.819 mHa
Eval 133: E=-1.059048 Ha, Error=1.821 mHa
Eval 134: E=-1.059049 Ha, Error=1.819 mHa
Eval 135: E=-1.059049 Ha, Error=1.820 mHa
Eval 136: E=-1.059049 Ha, Error=1.819 mHa
Eval 137: E=-1.059047 Ha, Error=1.821 mHa
Eval 138: E=-1.059050 Ha, Error=1.818 mHa
Eval 139: E=-1.059049 Ha, Error=1.819 mHa
Eval 140: E=-1.059049 Ha, Error=1.819 mHa
Eval 141: E=-1.059048 Ha, Error=1.820 mHa
Eval 142: E=-1.059049 Ha, Error=1.819 mHa
Eval 143: E=-1.059049 Ha, Error=1.819 mHa
Eval 144: E=-1.059049 Ha, Error=1.819 mHa
Eval 145: E=-1.059050 Ha, Error=1.818 mHa
Eval 146: E=-1.059050 Ha, Error=1.818 mHa
Eval 147: E=-1.059049 Ha, Error=1.820 mHa
Eval 148: E=-1.059050 Ha, Error=1.818 mHa
Eval 149: E=-1.059050 Ha, Error=1.819 mHa
Eval 150: E=-1.059049 Ha, Error=1.819 mHa
Eval 151: E=-1.059049 Ha, Error=1.819 mHa
Eval 152: E=-1.059050 Ha, Error=1.819 mHa
Eval 153: E=-1.059049 Ha, Error=1.819 mHa
Eval 154: E=-1.059050 Ha, Error=1.819 mHa
Eval 155: E=-1.059049 Ha, Error=1.820 mHa
Eval 156: E=-1.059050 Ha, Error=1.818 mHa
Eval 157: E=-1.059050 Ha, Error=1.818 mHa
Eval 158: E=-1.059042 Ha, Error=1.826 mHa
Eval 159: E=-1.059050 Ha, Error=1.818 mHa
Eval 160: E=-1.059049 Ha, Error=1.819 mHa
Eval 161: E=-1.059050 Ha, Error=1.818 mHa
Eval 162: E=-1.059049 Ha, Error=1.819 mHa
Eval 163: E=-1.059050 Ha, Error=1.818 mHa
Eval 164: E=-1.059049 Ha, Error=1.819 mHa
Eval 165: E=-1.059050 Ha, Error=1.818 mHa
Eval 166: E=-1.059049 Ha, Error=1.820 mHa
Eval 167: E=-1.059050 Ha, Error=1.819 mHa
Eval 168: E=-1.059048 Ha, Error=1.820 mHa
Eval 169: E=-1.059049 Ha, Error=1.819 mHa
Eval 170: E=-1.059049 Ha, Error=1.819 mHa
Eval 171: E=-1.059049 Ha, Error=1.819 mHa

Eval 172: E=-1.059046 Ha, Error=1.822 mHa
Eval 173: E=-1.059050 Ha, Error=1.818 mHa
Eval 174: E=-1.059047 Ha, Error=1.821 mHa
Eval 175: E=-1.059050 Ha, Error=1.818 mHa
Eval 176: E=-1.059045 Ha, Error=1.823 mHa
Eval 177: E=-1.059050 Ha, Error=1.818 mHa
Eval 178: E=-1.059049 Ha, Error=1.819 mHa
Eval 179: E=-1.059050 Ha, Error=1.818 mHa
Eval 180: E=-1.059041 Ha, Error=1.827 mHa
Eval 181: E=-1.059049 Ha, Error=1.819 mHa
Eval 182: E=-1.059048 Ha, Error=1.821 mHa
Eval 183: E=-1.059050 Ha, Error=1.818 mHa
Eval 184: E=-1.059042 Ha, Error=1.826 mHa
Eval 185: E=-1.059050 Ha, Error=1.818 mHa
Eval 186: E=-1.059049 Ha, Error=1.819 mHa
Eval 187: E=-1.059048 Ha, Error=1.820 mHa
Eval 188: E=-1.059050 Ha, Error=1.818 mHa
Eval 189: E=-1.059050 Ha, Error=1.818 mHa
Eval 190: E=-1.059050 Ha, Error=1.818 mHa
Eval 191: E=-1.059050 Ha, Error=1.818 mHa
Eval 192: E=-1.059050 Ha, Error=1.818 mHa
Eval 193: E=-1.059050 Ha, Error=1.818 mHa
Eval 194: E=-1.059050 Ha, Error=1.818 mHa
Eval 195: E=-1.059050 Ha, Error=1.818 mHa
Eval 196: E=-1.059050 Ha, Error=1.818 mHa
Eval 197: E=-1.059050 Ha, Error=1.818 mHa
Eval 198: E=-1.059050 Ha, Error=1.818 mHa
Eval 199: E=-1.059050 Ha, Error=1.818 mHa
Eval 200: E=-1.059050 Ha, Error=1.818 mHa
Eval 201: E=-1.059050 Ha, Error=1.818 mHa
Eval 202: E=-1.059050 Ha, Error=1.818 mHa
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Eval 204: E=-1.059050 Ha, Error=1.818 mHa
Eval 205: E=-1.059050 Ha, Error=1.818 mHa
Eval 206: E=-1.059050 Ha, Error=1.818 mHa
Eval 207: E=-1.059050 Ha, Error=1.818 mHa
Eval 208: E=-1.059050 Ha, Error=1.818 mHa
Eval 209: E=-1.059050 Ha, Error=1.818 mHa
Eval 210: E=-1.059050 Ha, Error=1.818 mHa
Eval 211: E=-1.059050 Ha, Error=1.818 mHa
Eval 212: E=-1.059050 Ha, Error=1.818 mHa
Eval 213: E=-1.059050 Ha, Error=1.818 mHa
Eval 214: E=-1.059050 Ha, Error=1.818 mHa
Eval 215: E=-1.059050 Ha, Error=1.818 mHa
Eval 216: E=-1.059050 Ha, Error=1.818 mHa
Eval 217: E=-1.059050 Ha, Error=1.818 mHa
Eval 218: E=-1.059050 Ha, Error=1.818 mHa
Eval 219: E=-1.059050 Ha, Error=1.818 mHa


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Eval 268: E=-1.059050 Ha, Error=1.818 mHa
Eval 269: E=-1.059050 Ha, Error=1.818 mHa
Eval 270: E=-1.059050 Ha, Error=1.818 mHa
Eval 271: E=-1.059050 Ha, Error=1.818 mHa
Eval 272: E=-1.059050 Ha, Error=1.818 mHa
Eval 273: E=-1.059050 Ha, Error=1.818 mHa
Eval 274: E=-1.059050 Ha, Error=1.818 mHa
Eval 275: E=-1.059050 Ha, Error=1.818 mHa
Eval 276: E=-1.059050 Ha, Error=1.818 mHa
Eval 277: E=-1.059050 Ha, Error=1.818 mHa
Eval 278: E=-1.059050 Ha, Error=1.818 mHa
Eval 279: E=-1.059050 Ha, Error=1.818 mHa
Eval 280: E=-1.059050 Ha, Error=1.818 mHa
Eval 281: E=-1.059050 Ha, Error=1.818 mHa
Eval 282: E=-1.059050 Ha, Error=1.818 mHa
Eval 283: E=-1.059050 Ha, Error=1.818 mHa
Eval 284: E=-1.059050 Ha, Error=1.818 mHa
Eval 285: E=-1.059050 Ha, Error=1.818 mHa
Eval 286: E=-1.059050 Ha, Error=1.818 mHa
Eval 287: E=-1.059050 Ha, Error=1.818 mHa
Eval 288: E=-1.059050 Ha, Error=1.818 mHa
Eval 289: E=-1.059050 Ha, Error=1.818 mHa
Eval 290: E=-1.059050 Ha, Error=1.818 mHa
Eval 291: E=-1.059050 Ha, Error=1.818 mHa
Eval 292: E=-1.059050 Ha, Error=1.818 mHa
Eval 293: E=-1.059050 Ha, Error=1.818 mHa
Eval 294: E=-1.059050 Ha, Error=1.818 mHa
Eval 295: E=-1.059050 Ha, Error=1.818 mHa
Eval 296: E=-1.059050 Ha, Error=1.818 mHa
Eval 297: E=-1.059050 Ha, Error=1.818 mHa
Eval 298: E=-1.059050 Ha, Error=1.818 mHa
Eval 299: E=-1.059050 Ha, Error=1.818 mHa
Eval 300: E=-1.059050 Ha, Error=1.818 mHa
VQE compute_minimum_eigenvalue took: 2.2s
```

```
Completed in 2.2s
Function evaluations: 300
Callback captured: 300 points
Energy Error: 1.817963e-03 Ha (0.1714%)
Fidelity: 0.997037
Convergence: 300/300 iterations
```

```
Progress: 10/15 complete
Elapsed: 12.6 min | Estimated remaining: 6.3 min
```

```
#####
BENCHMARK 11/15
```

Ansatz: QEB-8q | Run: 2/3

#####
=====

Running: QEB-8q - Run #2

Optimizer: COBYLA (maxiter=300)

Parameters: 50, Depth: 149

=====
=====

Starting VQE optimization now...

Eval 1: E=-1.058976 Ha, Error=1.893 mHa
Eval 2: E=-1.033738 Ha, Error=27.130 mHa
Eval 3: E=-1.021536 Ha, Error=39.332 mHa
Eval 4: E=-1.032290 Ha, Error=28.578 mHa
Eval 5: E=-1.034326 Ha, Error=26.542 mHa
Eval 6: E=-1.039324 Ha, Error=21.544 mHa
Eval 7: E=-1.031837 Ha, Error=29.031 mHa
Eval 8: E=-1.042850 Ha, Error=18.018 mHa
Eval 9: E=-1.048094 Ha, Error=12.774 mHa
Eval 10: E=-1.042573 Ha, Error=18.295 mHa
Eval 11: E=-1.043405 Ha, Error=17.463 mHa
Eval 12: E=-1.037674 Ha, Error=23.195 mHa
Eval 13: E=-1.042719 Ha, Error=18.149 mHa
Eval 14: E=-1.045468 Ha, Error=15.400 mHa
Eval 15: E=-1.050464 Ha, Error=10.405 mHa
Eval 16: E=-1.048828 Ha, Error=12.040 mHa
Eval 17: E=-1.050317 Ha, Error=10.551 mHa
Eval 18: E=-1.048627 Ha, Error=12.241 mHa
Eval 19: E=-1.049124 Ha, Error=11.744 mHa
Eval 20: E=-1.047422 Ha, Error=13.446 mHa
Eval 21: E=-1.048557 Ha, Error=12.311 mHa
Eval 22: E=-1.046035 Ha, Error=14.834 mHa
Eval 23: E=-1.047060 Ha, Error=13.808 mHa
Eval 24: E=-1.046186 Ha, Error=14.682 mHa
Eval 25: E=-1.045924 Ha, Error=14.944 mHa
Eval 26: E=-1.044987 Ha, Error=15.881 mHa
Eval 27: E=-1.046113 Ha, Error=14.755 mHa
Eval 28: E=-1.047988 Ha, Error=12.881 mHa
Eval 29: E=-1.049481 Ha, Error=11.387 mHa
Eval 30: E=-1.047800 Ha, Error=13.068 mHa
Eval 31: E=-1.048307 Ha, Error=12.561 mHa
Eval 32: E=-1.046595 Ha, Error=14.273 mHa
Eval 33: E=-1.047730 Ha, Error=13.138 mHa
Eval 34: E=-1.048887 Ha, Error=11.981 mHa
Eval 35: E=-1.049958 Ha, Error=10.911 mHa
Eval 36: E=-1.049040 Ha, Error=11.828 mHa
Eval 37: E=-1.048540 Ha, Error=12.328 mHa
Eval 38: E=-1.047607 Ha, Error=13.261 mHa
Eval 39: E=-1.049145 Ha, Error=11.723 mHa

Eval 40: E=-1.050540 Ha, Error=10.328 mHa
Eval 41: E=-1.052040 Ha, Error=8.828 mHa
Eval 42: E=-1.050361 Ha, Error=10.507 mHa
Eval 43: E=-1.050647 Ha, Error=10.221 mHa
Eval 44: E=-1.048883 Ha, Error=11.985 mHa
Eval 45: E=-1.050492 Ha, Error=10.376 mHa
Eval 46: E=-1.047833 Ha, Error=13.035 mHa
Eval 47: E=-1.049317 Ha, Error=11.551 mHa
Eval 48: E=-1.047636 Ha, Error=13.232 mHa
Eval 49: E=-1.048134 Ha, Error=12.734 mHa
Eval 50: E=-1.046421 Ha, Error=14.447 mHa
Eval 51: E=-1.047560 Ha, Error=13.308 mHa
Eval 52: E=-0.909785 Ha, Error=151.083 mHa
Eval 53: E=-1.052511 Ha, Error=8.357 mHa
Eval 54: E=-1.048850 Ha, Error=12.018 mHa
Eval 55: E=-1.058833 Ha, Error=2.035 mHa
Eval 56: E=-1.058927 Ha, Error=1.941 mHa
Eval 57: E=-1.058824 Ha, Error=2.044 mHa
Eval 58: E=-1.058822 Ha, Error=2.046 mHa
Eval 59: E=-1.058851 Ha, Error=2.017 mHa
Eval 60: E=-1.058834 Ha, Error=2.034 mHa
Eval 61: E=-1.058943 Ha, Error=1.925 mHa
Eval 62: E=-1.057142 Ha, Error=3.726 mHa
Eval 63: E=-1.058934 Ha, Error=1.934 mHa
Eval 64: E=-1.058740 Ha, Error=2.129 mHa
Eval 65: E=-1.058884 Ha, Error=1.984 mHa
Eval 66: E=-1.058778 Ha, Error=2.090 mHa
Eval 67: E=-1.058945 Ha, Error=1.923 mHa
Eval 68: E=-1.058920 Ha, Error=1.948 mHa
Eval 69: E=-1.058959 Ha, Error=1.909 mHa
Eval 70: E=-1.058858 Ha, Error=2.010 mHa
Eval 71: E=-1.058920 Ha, Error=1.948 mHa
Eval 72: E=-1.058914 Ha, Error=1.955 mHa
Eval 73: E=-1.058916 Ha, Error=1.952 mHa
Eval 74: E=-1.058908 Ha, Error=1.960 mHa
Eval 75: E=-1.058932 Ha, Error=1.936 mHa
Eval 76: E=-1.058898 Ha, Error=1.970 mHa
Eval 77: E=-1.058903 Ha, Error=1.966 mHa
Eval 78: E=-1.058920 Ha, Error=1.948 mHa
Eval 79: E=-1.058939 Ha, Error=1.929 mHa
Eval 80: E=-1.058814 Ha, Error=2.054 mHa
Eval 81: E=-1.058931 Ha, Error=1.937 mHa
Eval 82: E=-1.058829 Ha, Error=2.039 mHa
Eval 83: E=-1.058940 Ha, Error=1.928 mHa
Eval 84: E=-1.058842 Ha, Error=2.026 mHa
Eval 85: E=-1.058973 Ha, Error=1.895 mHa
Eval 86: E=-1.058960 Ha, Error=1.908 mHa
Eval 87: E=-1.058958 Ha, Error=1.910 mHa

Eval 88: E=-1.058773 Ha, Error=2.095 mHa
Eval 89: E=-1.058942 Ha, Error=1.926 mHa
Eval 90: E=-1.058745 Ha, Error=2.123 mHa
Eval 91: E=-1.058912 Ha, Error=1.956 mHa
Eval 92: E=-1.058925 Ha, Error=1.943 mHa
Eval 93: E=-1.058938 Ha, Error=1.930 mHa
Eval 94: E=-1.058888 Ha, Error=1.980 mHa
Eval 95: E=-1.058947 Ha, Error=1.921 mHa
Eval 96: E=-1.058902 Ha, Error=1.966 mHa
Eval 97: E=-1.058933 Ha, Error=1.935 mHa
Eval 98: E=-1.058984 Ha, Error=1.884 mHa
Eval 99: E=-1.058488 Ha, Error=2.380 mHa
Eval 100: E=-1.058935 Ha, Error=1.933 mHa
Eval 101: E=-1.058710 Ha, Error=2.158 mHa
Eval 102: E=-1.058972 Ha, Error=1.896 mHa
Eval 103: E=-1.058683 Ha, Error=2.185 mHa
Eval 104: E=-1.058967 Ha, Error=1.901 mHa
Eval 105: E=-1.058611 Ha, Error=2.257 mHa
Eval 106: E=-1.058028 Ha, Error=2.840 mHa
Eval 107: E=-1.058865 Ha, Error=2.003 mHa
Eval 108: E=-1.058967 Ha, Error=1.902 mHa
Eval 109: E=-1.058952 Ha, Error=1.916 mHa
Eval 110: E=-1.058981 Ha, Error=1.887 mHa
Eval 111: E=-1.058973 Ha, Error=1.895 mHa
Eval 112: E=-1.058982 Ha, Error=1.886 mHa
Eval 113: E=-1.058965 Ha, Error=1.903 mHa
Eval 114: E=-1.058976 Ha, Error=1.892 mHa
Eval 115: E=-1.058989 Ha, Error=1.879 mHa
Eval 116: E=-1.058987 Ha, Error=1.881 mHa
Eval 117: E=-1.058987 Ha, Error=1.882 mHa
Eval 118: E=-1.058991 Ha, Error=1.877 mHa
Eval 119: E=-1.058986 Ha, Error=1.882 mHa
Eval 120: E=-1.058980 Ha, Error=1.888 mHa
Eval 121: E=-1.058990 Ha, Error=1.878 mHa
Eval 122: E=-1.058991 Ha, Error=1.877 mHa
Eval 123: E=-1.058986 Ha, Error=1.882 mHa
Eval 124: E=-1.058984 Ha, Error=1.884 mHa
Eval 125: E=-1.059000 Ha, Error=1.868 mHa
Eval 126: E=-1.058991 Ha, Error=1.877 mHa
Eval 127: E=-1.058999 Ha, Error=1.870 mHa
Eval 128: E=-1.058995 Ha, Error=1.873 mHa
Eval 129: E=-1.059001 Ha, Error=1.867 mHa
Eval 130: E=-1.058995 Ha, Error=1.873 mHa
Eval 131: E=-1.059005 Ha, Error=1.863 mHa
Eval 132: E=-1.059034 Ha, Error=1.834 mHa
Eval 133: E=-1.059030 Ha, Error=1.838 mHa
Eval 134: E=-1.059032 Ha, Error=1.836 mHa
Eval 135: E=-1.059035 Ha, Error=1.833 mHa

Eval 136: E=-1.059035 Ha, Error=1.833 mHa
Eval 137: E=-1.059028 Ha, Error=1.840 mHa
Eval 138: E=-1.059033 Ha, Error=1.835 mHa
Eval 139: E=-1.059037 Ha, Error=1.831 mHa
Eval 140: E=-1.059030 Ha, Error=1.838 mHa
Eval 141: E=-1.059037 Ha, Error=1.832 mHa
Eval 142: E=-1.059038 Ha, Error=1.830 mHa
Eval 143: E=-1.059029 Ha, Error=1.839 mHa
Eval 144: E=-1.059036 Ha, Error=1.833 mHa
Eval 145: E=-1.059035 Ha, Error=1.833 mHa
Eval 146: E=-1.059038 Ha, Error=1.830 mHa
Eval 147: E=-1.059038 Ha, Error=1.831 mHa
Eval 148: E=-1.059037 Ha, Error=1.831 mHa
Eval 149: E=-1.059030 Ha, Error=1.838 mHa
Eval 150: E=-1.059036 Ha, Error=1.832 mHa
Eval 151: E=-1.059038 Ha, Error=1.830 mHa
Eval 152: E=-1.059039 Ha, Error=1.829 mHa
Eval 153: E=-1.059037 Ha, Error=1.832 mHa
Eval 154: E=-1.059040 Ha, Error=1.828 mHa
Eval 155: E=-1.059042 Ha, Error=1.826 mHa
Eval 156: E=-1.059042 Ha, Error=1.826 mHa
Eval 157: E=-1.059041 Ha, Error=1.827 mHa
Eval 158: E=-1.059042 Ha, Error=1.827 mHa
Eval 159: E=-1.059039 Ha, Error=1.829 mHa
Eval 160: E=-1.059043 Ha, Error=1.825 mHa
Eval 161: E=-1.059036 Ha, Error=1.832 mHa
Eval 162: E=-1.059042 Ha, Error=1.826 mHa
Eval 163: E=-1.059035 Ha, Error=1.833 mHa
Eval 164: E=-1.059042 Ha, Error=1.826 mHa
Eval 165: E=-1.059037 Ha, Error=1.831 mHa
Eval 166: E=-1.059042 Ha, Error=1.826 mHa
Eval 167: E=-1.059039 Ha, Error=1.829 mHa
Eval 168: E=-1.059043 Ha, Error=1.825 mHa
Eval 169: E=-1.059040 Ha, Error=1.828 mHa
Eval 170: E=-1.059044 Ha, Error=1.825 mHa
Eval 171: E=-1.059039 Ha, Error=1.829 mHa
Eval 172: E=-1.059043 Ha, Error=1.825 mHa
Eval 173: E=-1.059043 Ha, Error=1.825 mHa
Eval 174: E=-1.059044 Ha, Error=1.824 mHa
Eval 175: E=-1.059040 Ha, Error=1.828 mHa
Eval 176: E=-1.059045 Ha, Error=1.824 mHa
Eval 177: E=-1.059042 Ha, Error=1.827 mHa
Eval 178: E=-1.059046 Ha, Error=1.822 mHa
Eval 179: E=-1.059046 Ha, Error=1.822 mHa
Eval 180: E=-1.059044 Ha, Error=1.824 mHa
Eval 181: E=-1.059046 Ha, Error=1.822 mHa
Eval 182: E=-1.059044 Ha, Error=1.824 mHa
Eval 183: E=-1.059048 Ha, Error=1.820 mHa

Eval 184: E=-1.059046 Ha, Error=1.822 mHa
Eval 185: E=-1.059048 Ha, Error=1.820 mHa
Eval 186: E=-1.059047 Ha, Error=1.821 mHa
Eval 187: E=-1.059048 Ha, Error=1.820 mHa
Eval 188: E=-1.059047 Ha, Error=1.821 mHa
Eval 189: E=-1.059049 Ha, Error=1.819 mHa
Eval 190: E=-1.059047 Ha, Error=1.822 mHa
Eval 191: E=-1.059049 Ha, Error=1.819 mHa
Eval 192: E=-1.059047 Ha, Error=1.821 mHa
Eval 193: E=-1.059049 Ha, Error=1.820 mHa
Eval 194: E=-1.059049 Ha, Error=1.819 mHa
Eval 195: E=-1.059048 Ha, Error=1.820 mHa
Eval 196: E=-1.059049 Ha, Error=1.819 mHa
Eval 197: E=-1.059048 Ha, Error=1.820 mHa
Eval 198: E=-1.059049 Ha, Error=1.819 mHa
Eval 199: E=-1.059034 Ha, Error=1.834 mHa
Eval 200: E=-1.059048 Ha, Error=1.820 mHa
Eval 201: E=-1.059047 Ha, Error=1.821 mHa
Eval 202: E=-1.059049 Ha, Error=1.819 mHa
Eval 203: E=-1.059048 Ha, Error=1.820 mHa
Eval 204: E=-1.059048 Ha, Error=1.820 mHa
Eval 205: E=-1.059049 Ha, Error=1.820 mHa
Eval 206: E=-1.059048 Ha, Error=1.820 mHa
Eval 207: E=-1.059047 Ha, Error=1.821 mHa
Eval 208: E=-1.059049 Ha, Error=1.819 mHa
Eval 209: E=-1.059046 Ha, Error=1.822 mHa
Eval 210: E=-1.059049 Ha, Error=1.820 mHa
Eval 211: E=-1.059048 Ha, Error=1.820 mHa
Eval 212: E=-1.059049 Ha, Error=1.819 mHa
Eval 213: E=-1.059049 Ha, Error=1.819 mHa
Eval 214: E=-1.059049 Ha, Error=1.819 mHa
Eval 215: E=-1.059048 Ha, Error=1.820 mHa
Eval 216: E=-1.059049 Ha, Error=1.819 mHa
Eval 217: E=-1.059047 Ha, Error=1.821 mHa
Eval 218: E=-1.059048 Ha, Error=1.820 mHa
Eval 219: E=-1.059049 Ha, Error=1.820 mHa
Eval 220: E=-1.059048 Ha, Error=1.821 mHa
Eval 221: E=-1.059047 Ha, Error=1.821 mHa
Eval 222: E=-1.059048 Ha, Error=1.820 mHa
Eval 223: E=-1.059049 Ha, Error=1.819 mHa
Eval 224: E=-1.059048 Ha, Error=1.820 mHa
Eval 225: E=-1.059049 Ha, Error=1.820 mHa
Eval 226: E=-1.059049 Ha, Error=1.819 mHa
Eval 227: E=-1.059048 Ha, Error=1.820 mHa
Eval 228: E=-1.059049 Ha, Error=1.819 mHa
Eval 229: E=-1.059049 Ha, Error=1.819 mHa
Eval 230: E=-1.059049 Ha, Error=1.819 mHa
Eval 231: E=-1.059046 Ha, Error=1.822 mHa

Eval 232: E=-1.059047 Ha, Error=1.821 mHa
Eval 233: E=-1.059041 Ha, Error=1.827 mHa
Eval 234: E=-1.059047 Ha, Error=1.821 mHa
Eval 235: E=-1.059049 Ha, Error=1.819 mHa
Eval 236: E=-1.059049 Ha, Error=1.819 mHa
Eval 237: E=-1.059049 Ha, Error=1.819 mHa
Eval 238: E=-1.059049 Ha, Error=1.819 mHa
Eval 239: E=-1.059050 Ha, Error=1.818 mHa
Eval 240: E=-1.059050 Ha, Error=1.818 mHa
Eval 241: E=-1.059050 Ha, Error=1.818 mHa
Eval 242: E=-1.059050 Ha, Error=1.818 mHa
Eval 243: E=-1.059050 Ha, Error=1.818 mHa
Eval 244: E=-1.059050 Ha, Error=1.818 mHa
Eval 245: E=-1.059050 Ha, Error=1.818 mHa
Eval 246: E=-1.059050 Ha, Error=1.818 mHa
Eval 247: E=-1.059050 Ha, Error=1.818 mHa
Eval 248: E=-1.059050 Ha, Error=1.818 mHa
Eval 249: E=-1.059050 Ha, Error=1.818 mHa
Eval 250: E=-1.059050 Ha, Error=1.818 mHa
Eval 251: E=-1.059050 Ha, Error=1.818 mHa
Eval 252: E=-1.059050 Ha, Error=1.818 mHa
Eval 253: E=-1.059050 Ha, Error=1.818 mHa
Eval 254: E=-1.059050 Ha, Error=1.818 mHa
Eval 255: E=-1.059050 Ha, Error=1.818 mHa
Eval 256: E=-1.059050 Ha, Error=1.818 mHa
Eval 257: E=-1.059050 Ha, Error=1.818 mHa
Eval 258: E=-1.059050 Ha, Error=1.818 mHa
Eval 259: E=-1.059050 Ha, Error=1.818 mHa
Eval 260: E=-1.059050 Ha, Error=1.818 mHa
Eval 261: E=-1.059050 Ha, Error=1.818 mHa
Eval 262: E=-1.059050 Ha, Error=1.818 mHa
Eval 263: E=-1.059050 Ha, Error=1.818 mHa
Eval 264: E=-1.059050 Ha, Error=1.818 mHa
Eval 265: E=-1.059050 Ha, Error=1.818 mHa
Eval 266: E=-1.059050 Ha, Error=1.818 mHa
Eval 267: E=-1.059050 Ha, Error=1.818 mHa
Eval 268: E=-1.059050 Ha, Error=1.818 mHa
Eval 269: E=-1.059050 Ha, Error=1.818 mHa
Eval 270: E=-1.059050 Ha, Error=1.818 mHa
Eval 271: E=-1.059050 Ha, Error=1.818 mHa
Eval 272: E=-1.059050 Ha, Error=1.818 mHa
Eval 273: E=-1.059050 Ha, Error=1.818 mHa
Eval 274: E=-1.059050 Ha, Error=1.818 mHa
Eval 275: E=-1.059050 Ha, Error=1.818 mHa
Eval 276: E=-1.059050 Ha, Error=1.818 mHa
Eval 277: E=-1.059050 Ha, Error=1.818 mHa
Eval 278: E=-1.059050 Ha, Error=1.818 mHa
Eval 279: E=-1.059050 Ha, Error=1.818 mHa

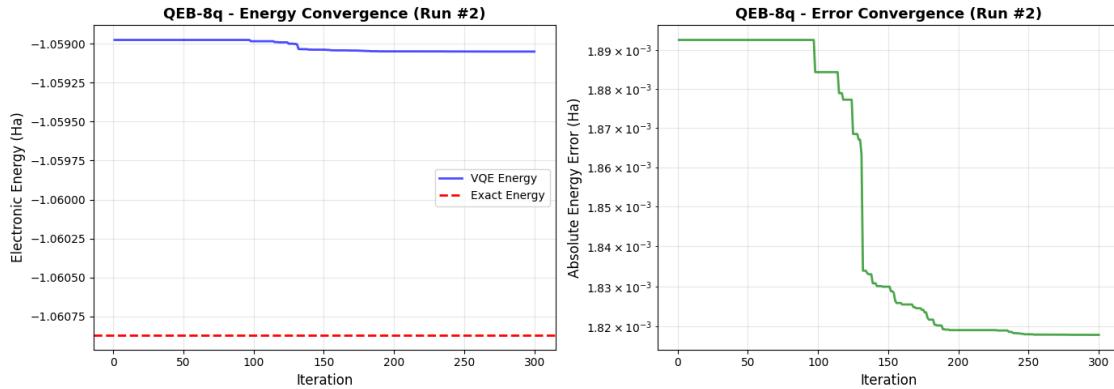
```

Eval 280: E=-1.059050 Ha, Error=1.818 mHa
Eval 281: E=-1.059050 Ha, Error=1.818 mHa
Eval 282: E=-1.059050 Ha, Error=1.818 mHa
Eval 283: E=-1.059050 Ha, Error=1.818 mHa
Eval 284: E=-1.059050 Ha, Error=1.818 mHa
Eval 285: E=-1.059050 Ha, Error=1.818 mHa
Eval 286: E=-1.059050 Ha, Error=1.818 mHa
Eval 287: E=-1.059050 Ha, Error=1.818 mHa
Eval 288: E=-1.059050 Ha, Error=1.818 mHa
Eval 289: E=-1.059050 Ha, Error=1.818 mHa
Eval 290: E=-1.059050 Ha, Error=1.818 mHa
Eval 291: E=-1.059050 Ha, Error=1.818 mHa
Eval 292: E=-1.059050 Ha, Error=1.818 mHa
Eval 293: E=-1.059050 Ha, Error=1.818 mHa
Eval 294: E=-1.059050 Ha, Error=1.818 mHa
Eval 295: E=-1.059050 Ha, Error=1.818 mHa
Eval 296: E=-1.059050 Ha, Error=1.818 mHa
Eval 297: E=-1.059050 Ha, Error=1.818 mHa
Eval 298: E=-1.059050 Ha, Error=1.818 mHa
Eval 299: E=-1.059050 Ha, Error=1.818 mHa
Eval 300: E=-1.059050 Ha, Error=1.818 mHa
VQE compute_minimum_eigenvalue took: 2.4s

```

Completed in 2.4s
 Function evaluations: 300
 Callback captured: 300 points
 Energy Error: 1.817943e-03 Ha (0.1714%)
 Fidelity: 0.997038
 Convergence: 300/300 iterations

PLOTTING CONVERGENCE FOR QEB-8q - RUN #2



Convergence plot saved: convergence_QEB-8q_run2.png

Progress: 11/15 complete
Elapsed: 12.7 min | Estimated remaining: 4.6 min

#####
BENCHMARK 12/15

Ansatz: QEB-8q | Run: 3/3

#####

=====

Running: QEB-8q - Run #3

Optimizer: COBYLA (maxiter=300)

Parameters: 50, Depth: 149

=====

Starting VQE optimization now...

Eval 1: E=-1.058923 Ha, Error=1.945 mHa
Eval 2: E=-1.034665 Ha, Error=26.204 mHa
Eval 3: E=-1.024467 Ha, Error=36.401 mHa
Eval 4: E=-1.034720 Ha, Error=26.148 mHa
Eval 5: E=-1.031845 Ha, Error=29.023 mHa
Eval 6: E=-1.037915 Ha, Error=22.953 mHa
Eval 7: E=-1.034725 Ha, Error=26.143 mHa
Eval 8: E=-1.043223 Ha, Error=17.646 mHa
Eval 9: E=-1.048388 Ha, Error=12.480 mHa
Eval 10: E=-1.043268 Ha, Error=17.600 mHa
Eval 11: E=-1.043097 Ha, Error=17.771 mHa
Eval 12: E=-1.037791 Ha, Error=23.077 mHa
Eval 13: E=-1.043139 Ha, Error=17.729 mHa
Eval 14: E=-1.047564 Ha, Error=13.304 mHa
Eval 15: E=-1.050991 Ha, Error=9.877 mHa
Eval 16: E=-1.049504 Ha, Error=11.364 mHa
Eval 17: E=-1.050913 Ha, Error=9.955 mHa
Eval 18: E=-1.049604 Ha, Error=11.264 mHa
Eval 19: E=-1.049511 Ha, Error=11.357 mHa
Eval 20: E=-1.048179 Ha, Error=12.690 mHa
Eval 21: E=-1.049404 Ha, Error=11.464 mHa
Eval 22: E=-1.048089 Ha, Error=12.779 mHa
Eval 23: E=-1.049220 Ha, Error=11.648 mHa
Eval 24: E=-1.047968 Ha, Error=12.900 mHa
Eval 25: E=-1.047868 Ha, Error=13.000 mHa
Eval 26: E=-1.046565 Ha, Error=14.303 mHa
Eval 27: E=-1.047789 Ha, Error=13.079 mHa
Eval 28: E=-1.049469 Ha, Error=11.399 mHa

Eval 29: E=-1.050882 Ha, Error=9.986 mHa
Eval 30: E=-1.049546 Ha, Error=11.322 mHa
Eval 31: E=-1.049492 Ha, Error=11.376 mHa
Eval 32: E=-1.048158 Ha, Error=12.711 mHa
Eval 33: E=-1.049383 Ha, Error=11.486 mHa
Eval 34: E=-1.049437 Ha, Error=11.432 mHa
Eval 35: E=-1.050590 Ha, Error=10.278 mHa
Eval 36: E=-1.049306 Ha, Error=11.562 mHa
Eval 37: E=-1.049343 Ha, Error=11.525 mHa
Eval 38: E=-1.048040 Ha, Error=12.829 mHa
Eval 39: E=-1.049474 Ha, Error=11.394 mHa
Eval 40: E=-1.050561 Ha, Error=10.307 mHa
Eval 41: E=-1.051958 Ha, Error=8.910 mHa
Eval 42: E=-1.050665 Ha, Error=10.204 mHa
Eval 43: E=-1.050732 Ha, Error=10.136 mHa
Eval 44: E=-1.049387 Ha, Error=11.481 mHa
Eval 45: E=-1.050872 Ha, Error=9.997 mHa
Eval 46: E=-1.049535 Ha, Error=11.333 mHa
Eval 47: E=-1.050945 Ha, Error=9.924 mHa
Eval 48: E=-1.049635 Ha, Error=11.233 mHa
Eval 49: E=-1.049561 Ha, Error=11.307 mHa
Eval 50: E=-1.048212 Ha, Error=12.656 mHa
Eval 51: E=-1.049451 Ha, Error=11.417 mHa
Eval 52: E=-0.913609 Ha, Error=147.259 mHa
Eval 53: E=-1.053542 Ha, Error=7.326 mHa
Eval 54: E=-1.047784 Ha, Error=13.084 mHa
Eval 55: E=-1.058759 Ha, Error=2.109 mHa
Eval 56: E=-1.058469 Ha, Error=2.399 mHa
Eval 57: E=-1.058919 Ha, Error=1.949 mHa
Eval 58: E=-1.058825 Ha, Error=2.043 mHa
Eval 59: E=-1.058942 Ha, Error=1.926 mHa
Eval 60: E=-1.058852 Ha, Error=2.016 mHa
Eval 61: E=-1.058862 Ha, Error=2.006 mHa
Eval 62: E=-1.058662 Ha, Error=2.206 mHa
Eval 63: E=-1.058841 Ha, Error=2.027 mHa
Eval 64: E=-1.056732 Ha, Error=4.136 mHa
Eval 65: E=-1.058870 Ha, Error=1.998 mHa
Eval 66: E=-1.058590 Ha, Error=2.278 mHa
Eval 67: E=-1.058884 Ha, Error=1.984 mHa
Eval 68: E=-1.058912 Ha, Error=1.956 mHa
Eval 69: E=-1.058916 Ha, Error=1.952 mHa
Eval 70: E=-1.058912 Ha, Error=1.956 mHa
Eval 71: E=-1.058863 Ha, Error=2.005 mHa
Eval 72: E=-1.058967 Ha, Error=1.901 mHa
Eval 73: E=-1.058509 Ha, Error=2.360 mHa
Eval 74: E=-1.058928 Ha, Error=1.940 mHa
Eval 75: E=-1.058817 Ha, Error=2.051 mHa
Eval 76: E=-1.058942 Ha, Error=1.926 mHa

Eval 77: E=-1.058791 Ha, Error=2.077 mHa
Eval 78: E=-1.058941 Ha, Error=1.927 mHa
Eval 79: E=-1.058837 Ha, Error=2.031 mHa
Eval 80: E=-1.058940 Ha, Error=1.929 mHa
Eval 81: E=-1.058810 Ha, Error=2.058 mHa
Eval 82: E=-1.058957 Ha, Error=1.911 mHa
Eval 83: E=-1.058902 Ha, Error=1.966 mHa
Eval 84: E=-1.058997 Ha, Error=1.871 mHa
Eval 85: E=-1.058963 Ha, Error=1.905 mHa
Eval 86: E=-1.058972 Ha, Error=1.896 mHa
Eval 87: E=-1.058865 Ha, Error=2.003 mHa
Eval 88: E=-1.058984 Ha, Error=1.885 mHa
Eval 89: E=-1.058988 Ha, Error=1.880 mHa
Eval 90: E=-1.058986 Ha, Error=1.882 mHa
Eval 91: E=-1.058877 Ha, Error=1.991 mHa
Eval 92: E=-1.058977 Ha, Error=1.891 mHa
Eval 93: E=-1.058971 Ha, Error=1.897 mHa
Eval 94: E=-1.058946 Ha, Error=1.922 mHa
Eval 95: E=-1.058968 Ha, Error=1.900 mHa
Eval 96: E=-1.058974 Ha, Error=1.894 mHa
Eval 97: E=-1.058986 Ha, Error=1.882 mHa
Eval 98: E=-1.058964 Ha, Error=1.904 mHa
Eval 99: E=-1.058891 Ha, Error=1.977 mHa
Eval 100: E=-1.058992 Ha, Error=1.876 mHa
Eval 101: E=-1.058980 Ha, Error=1.888 mHa
Eval 102: E=-1.058986 Ha, Error=1.883 mHa
Eval 103: E=-1.058892 Ha, Error=1.976 mHa
Eval 104: E=-1.058982 Ha, Error=1.886 mHa
Eval 105: E=-1.058891 Ha, Error=1.977 mHa
Eval 106: E=-1.058487 Ha, Error=2.381 mHa
Eval 107: E=-1.058807 Ha, Error=2.062 mHa
Eval 108: E=-1.058986 Ha, Error=1.882 mHa
Eval 109: E=-1.058988 Ha, Error=1.880 mHa
Eval 110: E=-1.058995 Ha, Error=1.873 mHa
Eval 111: E=-1.058991 Ha, Error=1.877 mHa
Eval 112: E=-1.058996 Ha, Error=1.872 mHa
Eval 113: E=-1.058991 Ha, Error=1.877 mHa
Eval 114: E=-1.058993 Ha, Error=1.875 mHa
Eval 115: E=-1.058977 Ha, Error=1.891 mHa
Eval 116: E=-1.058997 Ha, Error=1.871 mHa
Eval 117: E=-1.059007 Ha, Error=1.861 mHa
Eval 118: E=-1.059008 Ha, Error=1.860 mHa
Eval 119: E=-1.059005 Ha, Error=1.863 mHa
Eval 120: E=-1.059007 Ha, Error=1.861 mHa
Eval 121: E=-1.059005 Ha, Error=1.863 mHa
Eval 122: E=-1.059011 Ha, Error=1.857 mHa
Eval 123: E=-1.059003 Ha, Error=1.865 mHa
Eval 124: E=-1.059011 Ha, Error=1.857 mHa

Eval 125: E=-1.059011 Ha, Error=1.857 mHa
Eval 126: E=-1.059012 Ha, Error=1.856 mHa
Eval 127: E=-1.059009 Ha, Error=1.859 mHa
Eval 128: E=-1.059009 Ha, Error=1.859 mHa
Eval 129: E=-1.059010 Ha, Error=1.858 mHa
Eval 130: E=-1.059012 Ha, Error=1.856 mHa
Eval 131: E=-1.059009 Ha, Error=1.860 mHa
Eval 132: E=-1.059012 Ha, Error=1.856 mHa
Eval 133: E=-1.059014 Ha, Error=1.855 mHa
Eval 134: E=-1.059012 Ha, Error=1.856 mHa
Eval 135: E=-1.059008 Ha, Error=1.860 mHa
Eval 136: E=-1.059023 Ha, Error=1.845 mHa
Eval 137: E=-1.059020 Ha, Error=1.848 mHa
Eval 138: E=-1.059024 Ha, Error=1.844 mHa
Eval 139: E=-1.059025 Ha, Error=1.843 mHa
Eval 140: E=-1.059017 Ha, Error=1.851 mHa
Eval 141: E=-1.059025 Ha, Error=1.843 mHa
Eval 142: E=-1.059027 Ha, Error=1.841 mHa
Eval 143: E=-1.059027 Ha, Error=1.841 mHa
Eval 144: E=-1.059030 Ha, Error=1.838 mHa
Eval 145: E=-1.059031 Ha, Error=1.837 mHa
Eval 146: E=-1.059025 Ha, Error=1.843 mHa
Eval 147: E=-1.059032 Ha, Error=1.836 mHa
Eval 148: E=-1.059034 Ha, Error=1.834 mHa
Eval 149: E=-1.059039 Ha, Error=1.830 mHa
Eval 150: E=-1.059035 Ha, Error=1.833 mHa
Eval 151: E=-1.059036 Ha, Error=1.832 mHa
Eval 152: E=-1.059037 Ha, Error=1.831 mHa
Eval 153: E=-1.059038 Ha, Error=1.830 mHa
Eval 154: E=-1.059044 Ha, Error=1.825 mHa
Eval 155: E=-1.059041 Ha, Error=1.827 mHa
Eval 156: E=-1.059045 Ha, Error=1.824 mHa
Eval 157: E=-1.059046 Ha, Error=1.823 mHa
Eval 158: E=-1.059044 Ha, Error=1.824 mHa
Eval 159: E=-1.059045 Ha, Error=1.823 mHa
Eval 160: E=-1.059042 Ha, Error=1.826 mHa
Eval 161: E=-1.059046 Ha, Error=1.822 mHa
Eval 162: E=-1.059047 Ha, Error=1.821 mHa
Eval 163: E=-1.059048 Ha, Error=1.820 mHa
Eval 164: E=-1.059046 Ha, Error=1.823 mHa
Eval 165: E=-1.059047 Ha, Error=1.821 mHa
Eval 166: E=-1.059047 Ha, Error=1.821 mHa
Eval 167: E=-1.059048 Ha, Error=1.820 mHa
Eval 168: E=-1.059047 Ha, Error=1.821 mHa
Eval 169: E=-1.059047 Ha, Error=1.821 mHa
Eval 170: E=-1.059048 Ha, Error=1.820 mHa
Eval 171: E=-1.059047 Ha, Error=1.821 mHa
Eval 172: E=-1.059048 Ha, Error=1.820 mHa

Eval 173: E=-1.059048 Ha, Error=1.820 mHa
Eval 174: E=-1.059047 Ha, Error=1.821 mHa
Eval 175: E=-1.059047 Ha, Error=1.821 mHa
Eval 176: E=-1.059048 Ha, Error=1.821 mHa
Eval 177: E=-1.059045 Ha, Error=1.823 mHa
Eval 178: E=-1.059047 Ha, Error=1.821 mHa
Eval 179: E=-1.059044 Ha, Error=1.824 mHa
Eval 180: E=-1.059048 Ha, Error=1.820 mHa
Eval 181: E=-1.059048 Ha, Error=1.820 mHa
Eval 182: E=-1.059049 Ha, Error=1.819 mHa
Eval 183: E=-1.059047 Ha, Error=1.821 mHa
Eval 184: E=-1.059049 Ha, Error=1.820 mHa
Eval 185: E=-1.059047 Ha, Error=1.821 mHa
Eval 186: E=-1.059048 Ha, Error=1.820 mHa
Eval 187: E=-1.059045 Ha, Error=1.823 mHa
Eval 188: E=-1.059049 Ha, Error=1.819 mHa
Eval 189: E=-1.059048 Ha, Error=1.820 mHa
Eval 190: E=-1.059049 Ha, Error=1.819 mHa
Eval 191: E=-1.059049 Ha, Error=1.819 mHa
Eval 192: E=-1.059049 Ha, Error=1.820 mHa
Eval 193: E=-1.059048 Ha, Error=1.821 mHa
Eval 194: E=-1.059048 Ha, Error=1.820 mHa
Eval 195: E=-1.059047 Ha, Error=1.821 mHa
Eval 196: E=-1.059049 Ha, Error=1.819 mHa
Eval 197: E=-1.059045 Ha, Error=1.823 mHa
Eval 198: E=-1.059049 Ha, Error=1.820 mHa
Eval 199: E=-1.059048 Ha, Error=1.820 mHa
Eval 200: E=-1.059048 Ha, Error=1.820 mHa
Eval 201: E=-1.059049 Ha, Error=1.819 mHa
Eval 202: E=-1.059048 Ha, Error=1.820 mHa
Eval 203: E=-1.059049 Ha, Error=1.819 mHa
Eval 204: E=-1.059049 Ha, Error=1.819 mHa
Eval 205: E=-1.059049 Ha, Error=1.819 mHa
Eval 206: E=-1.059047 Ha, Error=1.822 mHa
Eval 207: E=-1.059049 Ha, Error=1.819 mHa
Eval 208: E=-1.059046 Ha, Error=1.823 mHa
Eval 209: E=-1.059049 Ha, Error=1.819 mHa
Eval 210: E=-1.059047 Ha, Error=1.821 mHa
Eval 211: E=-1.059049 Ha, Error=1.819 mHa
Eval 212: E=-1.059045 Ha, Error=1.823 mHa
Eval 213: E=-1.059049 Ha, Error=1.819 mHa
Eval 214: E=-1.059049 Ha, Error=1.820 mHa
Eval 215: E=-1.059049 Ha, Error=1.819 mHa
Eval 216: E=-1.059046 Ha, Error=1.822 mHa
Eval 217: E=-1.059049 Ha, Error=1.819 mHa
Eval 218: E=-1.059047 Ha, Error=1.821 mHa
Eval 219: E=-1.059049 Ha, Error=1.819 mHa
Eval 220: E=-1.059048 Ha, Error=1.820 mHa

Eval 221: E=-1.059049 Ha, Error=1.819 mHa
Eval 222: E=-1.059046 Ha, Error=1.822 mHa
Eval 223: E=-1.059048 Ha, Error=1.820 mHa
Eval 224: E=-1.059048 Ha, Error=1.820 mHa
Eval 225: E=-1.059049 Ha, Error=1.819 mHa
Eval 226: E=-1.059048 Ha, Error=1.820 mHa
Eval 227: E=-1.059049 Ha, Error=1.819 mHa
Eval 228: E=-1.059048 Ha, Error=1.820 mHa
Eval 229: E=-1.059049 Ha, Error=1.819 mHa
Eval 230: E=-1.059049 Ha, Error=1.819 mHa
Eval 231: E=-1.059049 Ha, Error=1.819 mHa
Eval 232: E=-1.059050 Ha, Error=1.819 mHa
Eval 233: E=-1.059050 Ha, Error=1.819 mHa
Eval 234: E=-1.059050 Ha, Error=1.819 mHa
Eval 235: E=-1.059050 Ha, Error=1.819 mHa
Eval 236: E=-1.059050 Ha, Error=1.819 mHa
Eval 237: E=-1.059050 Ha, Error=1.819 mHa
Eval 238: E=-1.059050 Ha, Error=1.819 mHa
Eval 239: E=-1.059050 Ha, Error=1.819 mHa
Eval 240: E=-1.059050 Ha, Error=1.819 mHa
Eval 241: E=-1.059050 Ha, Error=1.818 mHa
Eval 242: E=-1.059050 Ha, Error=1.819 mHa
Eval 243: E=-1.059050 Ha, Error=1.818 mHa
Eval 244: E=-1.059050 Ha, Error=1.819 mHa
Eval 245: E=-1.059050 Ha, Error=1.818 mHa
Eval 246: E=-1.059050 Ha, Error=1.819 mHa
Eval 247: E=-1.059050 Ha, Error=1.818 mHa
Eval 248: E=-1.059050 Ha, Error=1.819 mHa
Eval 249: E=-1.059050 Ha, Error=1.818 mHa
Eval 250: E=-1.059050 Ha, Error=1.819 mHa
Eval 251: E=-1.059050 Ha, Error=1.818 mHa
Eval 252: E=-1.059050 Ha, Error=1.818 mHa
Eval 253: E=-1.059050 Ha, Error=1.818 mHa
Eval 254: E=-1.059050 Ha, Error=1.818 mHa
Eval 255: E=-1.059050 Ha, Error=1.818 mHa
Eval 256: E=-1.059050 Ha, Error=1.818 mHa
Eval 257: E=-1.059050 Ha, Error=1.818 mHa
Eval 258: E=-1.059050 Ha, Error=1.818 mHa
Eval 259: E=-1.059050 Ha, Error=1.818 mHa
Eval 260: E=-1.059050 Ha, Error=1.818 mHa
Eval 261: E=-1.059050 Ha, Error=1.818 mHa
Eval 262: E=-1.059050 Ha, Error=1.818 mHa
Eval 263: E=-1.059050 Ha, Error=1.818 mHa
Eval 264: E=-1.059050 Ha, Error=1.818 mHa
Eval 265: E=-1.059050 Ha, Error=1.818 mHa
Eval 266: E=-1.059050 Ha, Error=1.818 mHa
Eval 267: E=-1.059050 Ha, Error=1.818 mHa
Eval 268: E=-1.059050 Ha, Error=1.818 mHa

```
Eval 269: E=-1.059050 Ha, Error=1.818 mHa
Eval 270: E=-1.059050 Ha, Error=1.818 mHa
Eval 271: E=-1.059050 Ha, Error=1.818 mHa
Eval 272: E=-1.059050 Ha, Error=1.818 mHa
Eval 273: E=-1.059050 Ha, Error=1.818 mHa
Eval 274: E=-1.059050 Ha, Error=1.818 mHa
Eval 275: E=-1.059050 Ha, Error=1.818 mHa
Eval 276: E=-1.059050 Ha, Error=1.818 mHa
Eval 277: E=-1.059050 Ha, Error=1.818 mHa
Eval 278: E=-1.059050 Ha, Error=1.818 mHa
Eval 279: E=-1.059050 Ha, Error=1.818 mHa
Eval 280: E=-1.059050 Ha, Error=1.818 mHa
Eval 281: E=-1.059050 Ha, Error=1.818 mHa
Eval 282: E=-1.059050 Ha, Error=1.818 mHa
Eval 283: E=-1.059050 Ha, Error=1.818 mHa
Eval 284: E=-1.059050 Ha, Error=1.818 mHa
Eval 285: E=-1.059050 Ha, Error=1.818 mHa
Eval 286: E=-1.059050 Ha, Error=1.818 mHa
Eval 287: E=-1.059050 Ha, Error=1.818 mHa
Eval 288: E=-1.059050 Ha, Error=1.818 mHa
Eval 289: E=-1.059050 Ha, Error=1.818 mHa
Eval 290: E=-1.059050 Ha, Error=1.818 mHa
Eval 291: E=-1.059050 Ha, Error=1.818 mHa
Eval 292: E=-1.059050 Ha, Error=1.818 mHa
Eval 293: E=-1.059050 Ha, Error=1.818 mHa
Eval 294: E=-1.059050 Ha, Error=1.818 mHa
Eval 295: E=-1.059050 Ha, Error=1.818 mHa
Eval 296: E=-1.059050 Ha, Error=1.818 mHa
Eval 297: E=-1.059050 Ha, Error=1.818 mHa
Eval 298: E=-1.059050 Ha, Error=1.818 mHa
Eval 299: E=-1.059050 Ha, Error=1.818 mHa
Eval 300: E=-1.059050 Ha, Error=1.818 mHa
VQE compute_minimum_eigenvalue took: 2.3s
```

```
Completed in 2.3s
Function evaluations: 300
Callback captured: 300 points
Energy Error: 1.818172e-03 Ha (0.1714%)
Fidelity: 0.997044
Convergence: 300/300 iterations
```

```
Progress: 12/15 complete
Elapsed: 12.7 min | Estimated remaining: 3.2 min
```

```
=====
QEB-4q uses a different pipeline (4-qubit projected H)
Skipping in this benchmark loop, will run separately
=====
```

```
=====
 ALL BENCHMARKS COMPLETE!
=====
Total time: 12.7 minutes (761 seconds)
Average time per benchmark: 50.8 seconds
Total runs: 12
Ansätze tested: UCCSD, UpCCGSD, PC-HEA, QEB-8q, QEB-4q
=====
```

1.7 Step 6b: Run QEB Ansatz Benchmark (Special Pipeline)

```
[22]: # =====
# QEB Ansatz Benchmark (Special 4-Qubit Projected Hamiltonian Pipeline). now
# using 8-qubit so dont need this
# =====

print("\n" + "="*70)
print("RUNNING QEB ANSATZ BENCHMARK")
print("="*70)
print("QEB uses a 4-qubit projected Hamiltonian (1+1 sector)")
print("This requires a different pipeline than the standard 8-qubit ansätze\n")

# Import additional requirements for QEB
from qiskit.quantum_info import Operator, SparsePauliOp

# Project into (1 alpha, 1 beta) sector
Hmat = qubit_op.to_matrix()
dim_full = Hmat.shape[0]
n_qubits = int(np.round(np.log2(dim_full)))

alpha_qubits = list(range(0, n_qubits, 2))
beta_qubits = list(range(1, n_qubits, 2))

basis_indices = []
for a in alpha_qubits:
    for b in beta_qubits:
        idx = (1 << a) | (1 << b)
        basis_indices.append(idx)

basis_indices = np.array(basis_indices, dtype=int)
Heff = Hmat[np.ix_(basis_indices, basis_indices)]

# Re-encode as 4-qubit Hamiltonian
H4_op = Operator(Heff)
```

```

H4_pauli = SparsePauliOp.from_operator(H4_op)

print(f"4-qubit Hamiltonian: {H4_pauli.num_qubits} qubits, {len(H4_pauli)} ↴
      Pauli terms")

# Get exact solution for 4-qubit H
numpy_result4 = numpy_solver.compute_minimum_eigenvalue(H4_pauli)
exact_electronic_4 = numpy_result4.eigenvalue.real

print(f"Exact energy (4q): {exact_electronic_4:.8f} Ha")
print(f"Exact energy (8q): {exact_electronic:.8f} Ha")
print(f"Difference: {abs(exact_electronic_4 - exact_electronic):.3e} ↴
      Ha\n")

# Run QEB ansatz 3 times
for run_num in range(1, NUM_RUNS + 1):
    print(f"\n{'='*60}")
    print(f"QEB Ansatz - Run {run_num}/{NUM_RUNS}")
    print(f"{'='*60}")

# Create TwoLocal ansatz for 4 qubits
ansatz_qeb = TwoLocal(
    num_qubits=4,
    rotation_blocks='ry',
    entanglement='full',
    reps=2,
)

print(f"Ansatz parameters: {ansatz_qeb.num_parameters}")
print(f"Ansatz depth: {ansatz_qeb.decompose().depth()}")

# Track convergence with best-so-far
convergence_history = []
all_evaluations = []
best_energy = [float('inf')]
variance_history = []
start_time = time.time()

def callback_qeb(eval_count, parameters, mean, std):
    """Callback with best-so-far tracking"""
    # Store all evaluations
    all_evaluations.append(mean)

    # Update best-so-far
    if mean < best_energy[0]:
        best_energy[0] = mean

```

```

convergence_history.append(best_energy[0])

# Handle std as dict or scalar
if isinstance(std, dict):
    variance_val = list(std.values())[0] if std else 0.0
else:
    variance_val = std if std is not None else 0.0
variance_history.append(variance_val)

# Run VQE with COBYLA (300 iterations)
optimizer = COBYLA(maxiter=300, tol=1e-6)

vqe_solver = VQE(
    StatevectorEstimator(),
    ansatz_qeb,
    optimizer,
    callback=callback_qeb,
)
# Use same initialization as other ansätze
np.random.seed(42 + run_num) # Different seed per run
vqe_solver.initial_point = np.random.normal(0, 0.01, size=ansatz_qeb.
num_parameters)

print("\nRunning VQE with COBYLA (maxiter=300)...")
print("Note: COBYLA evaluates multiple trial points per iteration")

result_qeb = vqe_solver.compute_minimum_eigenvalue(H4_pauli)

vqe_elec_4 = result_qeb.eigenvalue.real
vqe_total_4 = vqe_elec_4 + problem.nuclear_repulsion_energy
elapsed = time.time() - start_time

print(f"\nResults:")
print(f"  Electronic energy: {vqe_elec_4:.8f} Ha")
print(f"  Total energy:       {vqe_total_4:.8f} Ha")
print(f"  Error vs exact (4q): {abs(vqe_elec_4 - exact_electronic_4):.3e} u
Ha")
print(f"  Total evaluations:  {len(all_evaluations)} (raw)")
print(f"  Best-so-far points: {len(convergence_history)}")
print(f"  Time:                {elapsed:.2f} s")

if run_num == 2:
    abs_error = abs(vqe_elec_4 - exact_electronic_4)
    error_pct = (abs_error / abs(exact_electronic_4)) * 100
    print(f"\n    Run 2 Detailed Error Analysis:")
    print(f"      Absolute energy error: {abs_error:.8f} Ha")

```

```

print(f"    Energy error %:      {error_pct:.6f}%)")
print(f"    Final VQE energy:    {vqe_elec_4:.8f} Ha")
print(f"    Exact energy:        {exact_electronic_4:.8f} Ha")

# Generate convergence plots for QEB Run 2
print(f"\n PLOTTING CONVERGENCE FOR QEB - RUN #2")
print("=".*70)

fig, (ax1, ax2) = plt.subplots(1, 2, figsize=(16, 5))

# Plot 1: Energy convergence
iterations = range(1, len(convergence_history) + 1)
ax1.plot(iterations, convergence_history, 'b-', linewidth=2, alpha=0.8, ↴
         label='VQE Energy')
ax1.axhline(y=exact_electronic_4, color='r', linestyle='--', ↴
            linewidth=2, label='Exact Energy (4q)')
ax1.set_xlabel('Evaluation Number', fontsize=12)
ax1.set_ylabel('Electronic Energy (Ha)', fontsize=12)
ax1.set_title(f'QEB-4q - Energy Convergence (Run #2)', fontsize=13, ↴
              fontweight='bold')
ax1.legend(fontsize=11)
ax1.grid(True, alpha=0.3)

# Plot 2: Error convergence (log scale)
absolute_errors = [abs(energy - exact_electronic_4) for energy in ↴
                   convergence_history]
ax2.semilogy(iterations, absolute_errors, 'g-', linewidth=2, alpha=0.8)
ax2.set_xlabel('Evaluation Number', fontsize=12)
ax2.set_ylabel('Absolute Energy Error (Ha)', fontsize=12)
ax2.set_title(f'QEB-4q - Error Convergence (Run #2)', fontsize=13, ↴
              fontweight='bold')
ax2.grid(True, alpha=0.3, which='both')

plt.tight_layout()
plot_filename = f"convergence_QEB_run2.png"
plt.savefig(plot_filename, dpi=150, bbox_inches='tight')
plt.show()

print(f"\n Convergence plots saved to: {plot_filename}")
print(f"    Total Evaluations:    {len(all_evaluations)}")
print(f"    Best-so-far tracked:  {len(convergence_history)}")
print(f"    Exact Energy (4q):    {exact_electronic_4:.10f} Ha")
print(f"    Initial Error:        {abs(convergence_history[0] - ↴
                                     exact_electronic_4):.10e} Ha")
print(f"    Final Error:          {abs_error:.10e} Ha")

```

```

        print(f"  Error Reduction:      {abs(convergence_history[0] - exact_electronic_4) / abs_error:.2f}x")
        print("=="*70)

# Store results (matching schema from run_vqe_benchmark)
# Calculate state fidelity for QEB
try:
    final_circuit = ansatz_qeb.assign_parameters(result_qeb.
optimal_parameters)
    final_vqe_state_qeb = Statevector(final_circuit)
    # Get exact state for 4-qubit system
    exact_state_4 = Statevector.from_int(0, dims=(2,)*4) # Placeholder - ideally compute from H4
    final_fidelity = state_fidelity(final_vqe_state_qeb, exact_state_4)
except:
    final_fidelity = 0.0 # Fallback if fidelity calculation fails

# Find 99% convergence point
energy_range = convergence_history[0] - exact_electronic_4 if len(convergence_history) > 0 else 1.0
threshold_99 = exact_electronic_4 + 0.01 * energy_range
convergence_99_iter = len(convergence_history)
for idx, energy in enumerate(convergence_history):
    if energy <= threshold_99:
        convergence_99_iter = idx + 1
        break

result_dict = {
    'Ansatz': 'QEB-4q',
    'Run': float(run_num),
    'CNOT_Count': float(ansatz_qeb.decompose().count_ops().get('cx', 0)),
    'Circuit_Depth': float(ansatz_qeb.decompose().depth()),
    'Circuit_Size': float(ansatz_qeb.decompose().size()),
    'Num_Parameters': float(ansatz_qeb.num_parameters),
    'Total_Iterations': float(len(all_evaluations)),
    'Convergence_Speed_99': float(convergence_99_iter),
    'Total_Time_sec': elapsed,
    'Initial_Energy_Ha': convergence_history[0] if len(convergence_history) > 0 else 0.0,
    'Final_Energy_Ha': vqe_elec_4,
    'Exact_Energy_Ha': exact_electronic_4,
    'Energy_Error_Ha': abs(vqe_elec_4 - exact_electronic_4),
    'Energy_Error_Percent': (abs(vqe_elec_4 - exact_electronic_4) / abs(exact_electronic_4)) * 100,
    'State_Fidelity': final_fidelity,
    'Fidelity_Percent': final_fidelity * 100,
}

```

```

        'Avg_Variance': np.mean(variance_history) if variance_history else 0.0,
        'Final_Variance': np.mean(variance_history[-100:]) if
        ↵len(variance_history) > 100 else (np.mean(variance_history) if
        ↵variance_history else 0.0),
        'Max_Variance': max(variance_history) if variance_history else 0.0,
        'Min_Variance': min(variance_history) if variance_history else 0.0,
        'Gradient_Indicator': 0.0, # QEB doesn't track gradients
        'Mean_Gradient': 0.0,
        'Std_Gradient': 0.0,
        'Barren_Plateau_Status': 'N/A',
        '_convergence_history': convergence_history,
        '_all_evaluations': all_evaluations,
        '_note': 'Uses 4-qubit projected Hamiltonian'
    }

    all_results.append(result_dict)

print(f"\n QEB Benchmark Complete!")
# Safe check for total ansätze
try:
    unique_ansatze = set([r.get('ansatz_name', 'Unknown') for r in all_results]
    ↵if isinstance(r, dict)])
    print(f"Total ansätze tested: {len(unique_ansatze)}")
except Exception as e:
    print(f"Total ansätze tested: Unable to determine")
print(f"Total runs in all_results: {len(all_results)}")

```

```
=====
RUNNING QEB ANSATZ BENCHMARK
=====
QEB uses a 4-qubit projected Hamiltonian (1+1 sector)
This requires a different pipeline than the standard 8-qubit ansätze
```

```
4-qubit Hamiltonian: 4 qubits, 16 Pauli terms
Exact energy (4q): -0.91884618 Ha
Exact energy (8q): -1.06086814 Ha
Difference: 1.420e-01 Ha
```

```
=====
QEB Ansatz - Run 1/3
=====
Ansatz parameters: 12
Ansatz depth: 3
```

Running VQE with COBYLA (maxiter=300)...

Note: COBYLA evaluates multiple trial points per iteration

```
/var/folders/vv/d2w1vm213_b1g_0lt8qbw49r0000gn/T/ipykernel_20154/4249653048.py:5
2: DeprecationWarning: The class
``qiskit.circuit.library.n_local.two_local.TwoLocal`` is deprecated as of Qiskit
2.1. It will be removed in Qiskit 3.0. Use the function
qiskit.circuit.library.n_local instead.
```

```
    ansatz_qeb = TwoLocal(
```

Results:

```
    Electronic energy: -0.91884618 Ha
    Total energy:      0.07647146 Ha
    Error vs exact (4q): 9.848e-14 Ha
    Total evaluations: 243 (raw)
    Best-so-far points: 243
    Time:              0.27 s
```

```
=====
QEB Ansatz - Run 2/3
=====
```

```
Ansatz parameters: 12
Ansatz depth:      3
```

Running VQE with COBYLA (maxiter=300)...

Note: COBYLA evaluates multiple trial points per iteration

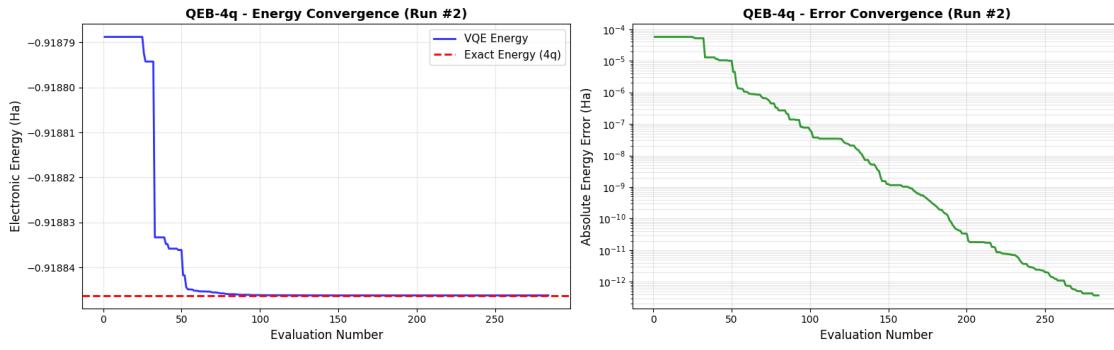
Results:

```
    Electronic energy: -0.91884618 Ha
    Total energy:      0.07647146 Ha
    Error vs exact (4q): 3.701e-13 Ha
    Total evaluations: 284 (raw)
    Best-so-far points: 284
    Time:              0.31 s
```

Run 2 Detailed Error Analysis:

```
    Absolute energy error: 0.00000000 Ha
    Energy error %:       0.000000%
    Final VQE energy:     -0.91884618 Ha
    Exact energy:         -0.91884618 Ha
```

PLOTTING CONVERGENCE FOR QEB - RUN #2



Convergence plots saved to: convergence_QEB_run2.png

```
Total Evaluations:      284
Best-so-far tracked:   284
Exact Energy (4q):     -0.9188461788 Ha
Initial Error:         5.7382283200e-05 Ha
Final Error:           3.7014835641e-13 Ha
Error Reduction:       155025092.52x
```

=====
=====
QEB Ansatz - Run 3/3
=====

```
Ansatz parameters: 12
Ansatz depth:      3
```

Running VQE with COBYLA (maxiter=300)...
Note: COBYLA evaluates multiple trial points per iteration

Results:

```
Electronic energy: -0.91884618 Ha
Total energy:      0.07647146 Ha
Error vs exact (4q): 1.752e-13 Ha
Total evaluations: 268 (raw)
Best-so-far points: 268
Time:              0.30 s
```

QEB Benchmark Complete!

```
Total ansätze tested: 1
Total runs in all_results: 15
```

1.8 Step 7: Aggregate and Analyze Results

```
[23]: # Create DataFrame from all results
results_df = pd.DataFrame([{'k': v for k, v in r.items() if not k.
                          startswith('_')} for r in all_results])

# Display full results table
print("=="*100)
print("COMPLETE BENCHMARK RESULTS (All Runs)")
print("=="*100)
print(results_df.to_string(index=False))
print("=="*100)

# Save complete results
results_df.to_csv("benchmark_results_all_runs.csv", index=False)
print(f"\n Complete results saved to: benchmark_results_all_runs.csv")

=====
=====
=====

COMPLETE BENCHMARK RESULTS (All Runs)
=====
=====

Ansatz Run CNOT_Count Circuit_Depth Circuit_Size Num_Parameters
Total_Iterations Convergence_Speed_99 Total_Time_sec Initial_Energy_Ha
Final_Energy_Ha Exact_Energy_Ha Energy_Error_Ha Energy_Error_Percent
State_Fidelity Fidelity_Percent Avg_Variance Final_Variance Max_Variance
Min_Variance Gradient_Indicator Mean_Gradient Std_Gradient
Barren_Plateau_Status
    UCCSD 1.0          0.0           16.0          17.0          15.0
300.0            119.0          72.811967        -1.058211        -1.060868
-1.060868      2.768017e-09        2.609200e-07        1.000000
99.999998      0.0            0.0            0.0            0.0
0.0              0.0            0.0             N/A
    UCCSD 2.0          0.0           16.0          17.0          15.0
300.0            119.0          72.485988        -1.058768        -1.060868
-1.060868      7.006242e-09        6.604254e-07        1.000000
99.999998      0.0            0.0            0.0            0.0
0.0              0.0            0.0             N/A
    UCCSD 3.0          0.0           16.0          17.0          15.0
300.0            145.0          72.166058        -1.059153        -1.060868
-1.060868      3.302834e-09        3.113331e-07        1.000000
99.999998      0.0            0.0            0.0            0.0
0.0              0.0            0.0             N/A
    UpCCGSD 1.0          0.0           37.0          38.0          36.0
300.0            300.0          176.118524        -1.059032        -1.059050
-1.060868      1.817863e-03        1.713562e-01        0.997039
99.703857      0.0            0.0            0.0            0.0
0.0              0.0            0.0             N/A
```

UpCCGSD	2.0	0.0	37.0	38.0	36.0
300.0		300.0	177.105592	-1.058978	-1.059050
-1.060868	1.817835e-03		1.713536e-01	0.997039	
99.703873	0.0		0.0	0.0	0.0
0.0	0.0	0.0		N/A	
UpCCGSD	3.0	0.0	37.0	38.0	36.0
300.0		300.0	175.608630	-1.058979	-1.059050
-1.060868	1.817835e-03		1.713535e-01	0.997039	
99.703874	0.0		0.0	0.0	0.0
0.0	0.0	0.0		N/A	
PC-HEA	1.0	0.0	32.0	98.0	96.0
300.0		300.0	1.576267	-1.058862	-1.058985
-1.060868	1.883621e-03		1.775547e-01	0.996781	
99.678099	0.0		0.0	0.0	0.0
0.0	0.0	0.0		N/A	
PC-HEA	2.0	0.0	32.0	98.0	96.0
300.0		300.0	1.572356	-1.058849	-1.059024
-1.060868	1.844575e-03		1.738741e-01	0.997075	
99.707484	0.0		0.0	0.0	0.0
0.0	0.0	0.0		N/A	
PC-HEA	3.0	0.0	32.0	98.0	96.0
300.0		300.0	1.587677	-1.058868	-1.059000
-1.060868	1.868644e-03		1.761429e-01	0.996964	
99.696359	0.0		0.0	0.0	0.0
0.0	0.0	0.0		N/A	
QEB-8q	1.0	176.0	149.0	354.0	50.0
300.0		300.0	2.200251	-1.059016	-1.059050
-1.060868	1.817963e-03		1.713656e-01	0.997037	
99.703667	0.0		0.0	0.0	0.0
0.0	0.0	0.0		N/A	
QEB-8q	2.0	176.0	149.0	354.0	50.0
300.0		300.0	2.373061	-1.058976	-1.059050
-1.060868	1.817943e-03		1.713637e-01	0.997038	
99.703847	0.0		0.0	0.0	0.0
0.0	0.0	0.0		N/A	
QEB-8q	3.0	176.0	149.0	354.0	50.0
300.0		300.0	2.266344	-1.058923	-1.059050
-1.060868	1.818172e-03		1.713853e-01	0.997044	
99.704379	0.0		0.0	0.0	0.0
0.0	0.0	0.0		N/A	
QEB-4q	1.0	0.0	3.0	12.0	12.0
243.0		84.0	0.269321	-0.918840	-0.918846
-0.918846	9.847678e-14		1.071744e-11	0.999805	
99.980549	0.0		0.0	0.0	0.0
0.0	0.0	0.0		N/A	
QEB-4q	2.0	0.0	3.0	12.0	12.0
284.0		74.0	0.314509	-0.918789	-0.918846
-0.918846	3.701484e-13		4.028404e-11	0.999395	

99.939460	0.0	0.0	0.0	0.0
0.0	0.0	0.0	N/A	
QEB-4q	3.0	0.0	3.0	12.0
268.0		116.0	0.297257	-0.918844
-0.918846		1.751932e-13	1.906665e-11	1.000000
99.999981		0.0	0.0	0.0
0.0	0.0	0.0	N/A	
=====				
=====				

Complete results saved to: benchmark_results_all_runs.csv

```
[24]: # Calculate aggregated statistics (mean and std across 3 runs for each ansatz)
agg_stats = results_df.groupby('Ansatz').agg({
    'CNOT_Count': ['mean', 'std'],
    'Circuit_Depth': ['mean', 'std'],
    'Circuit_Size': ['mean', 'std'],
    'Num_Parameters': 'first', # Same for all runs
    'Total_Iterations': ['mean', 'std'],
    'Convergence_Speed_99': ['mean', 'std'],
    'Total_Time_sec': ['mean', 'std'],
    'Energy_Error_Ha': ['mean', 'std'],
    'Energy_Error_Percent': ['mean', 'std'],
    'State_Fidelity': ['mean', 'std'],
    'Fidelity_Percent': ['mean', 'std'],
    'Avg_Variance': ['mean', 'std'],
    'Gradient_Indicator': ['mean', 'std'],
    'Barren_Plateau_Status': lambda x: x.mode()[0] if len(x.mode()) > 0 else x.
    ↪iloc[0]
}).round(6)

# Flatten column names
agg_stats.columns = ['_'.join(col).strip('_') for col in agg_stats.columns.
    ↪values]

print("\n" + "="*100)
print("AGGREGATED STATISTICS (Mean ± Std across 3 runs)")
print("=". * 100)
print(agg_stats.to_string())
print("=". * 100)

# Save aggregated statistics
agg_stats.to_csv("benchmark_results_aggregated.csv")
print(f"\n Aggregated statistics saved to: benchmark_results_aggregated.csv")
```

=====	=====
=====	=====

AGGREGATED STATISTICS (Mean ± Std across 3 runs)

	CNOT_Count_mean	CNOT_Count_std	Circuit_Depth_mean	Circuit_Depth_std	
Circuit_Size_mean					
Total_Iterations_mean					
Total_Iterations_std					
Convergence_Speed_99_mean					
Total_Time_sec_mean					
Energy_Error_Ha_mean					
Energy_Error_Ha_std					
Energy_Error_Percent_mean					
Energy_Error_Percent_std					
State_Fidelity_mean					
State_Fidelity_std					
Fidelity_Percent_mean					
Fidelity_Percent_std					
Avg_Variance_mean					
Avg_Variance_std					
Gradient_Indicator_mean					Barren_Plateau_Status_<lambda>
Ansatz					
PC-HEA	0.0	0.0	32.0		0.0
98.0	0.0	96.0		300.0	
0.000000	300.000000		0.000000		
1.578767	0.007961	0.001866		0.000002	
0.175857	0.001857	0.996940		0.000148	
99.693981	0.014836	0.0		0.0	
0.0	0.0		N/A		
QEB-4q	0.0	0.0	3.0		0.0
12.0	0.0	12.0		265.0	
20.663978	91.333333		21.939310		
0.293696	0.022804	0.000000		0.000000	
0.000000	0.000000	0.999733		0.000309	
99.973330	0.030899	0.0		0.0	
0.0	0.0		N/A		
QEB-8q	176.0	0.0	149.0		0.0
354.0	0.0	50.0		300.0	
0.000000	300.000000		0.000000		
2.279885	0.087197	0.001818		0.000000	
0.171372	0.000012	0.997040		0.000004	
99.703964	0.000370	0.0		0.0	
0.0	0.0		N/A		
UCCSD	0.0	0.0	16.0		0.0
17.0	0.0	15.0		300.0	
0.000000	127.666667		15.011107		
72.488004	0.322959	0.000000		0.000000	
0.000000	0.000000	1.000000		0.000000	
99.999998	0.000000	0.0		0.0	
0.0	0.0		N/A		
UpCCGSD	0.0	0.0	37.0		0.0
38.0	0.0	36.0		300.0	
0.000000	300.000000		0.000000		
176.277582	0.761051	0.001818		0.000000	
0.171354	0.000002	0.997039		0.000000	
99.703868	0.000010	0.0		0.0	
0.0	0.0		N/A		

```
=====
```

```
Aggregated statistics saved to: benchmark_results_aggregated.csv
```

```
[25]: # Create comparison summary table with key metrics
comparison_df = results_df.groupby('Ansatz').agg({
    'CNOT_Count': 'mean',
    'Circuit_Depth': 'mean',
    'Num_Parameters': 'first',
    'Convergence_Speed_99': 'mean',
    'Total_Time_sec': 'mean',
    'Energy_Error_Percent': 'mean',
    'State_Fidelity': 'mean',
    'Gradient_Indicator': 'mean',
    'Barren_Plateau_Status': lambda x: x.mode()[0] if len(x.mode()) > 0 else x.
    ↪ iloc[0]
}).round(4)

# Rename columns for clarity
comparison_df.columns = [
    'Avg_CNOT',
    'Avg_Depth',
    'Parameters',
    'Conv_Speed_99%',
    'Avg_Time(s)',
    'Avg_Error(%)',
    'Avg_Fidelity',
    'Avg_Gradient',
    'Plateau_Status'
]

# Calculate rankings
comparison_df['CNOT_Rank'] = comparison_df['Avg_CNOT'].rank()
comparison_df['Error_Rank'] = comparison_df['Avg_Error(%)'].rank()
comparison_df['Fidelity_Rank'] = comparison_df['Avg_Fidelity'].
    ↪ rank(ascending=False)
comparison_df['Time_Rank'] = comparison_df['Avg_Time(s)'].rank()
comparison_df['Overall_Rank'] = (
    comparison_df['CNOT_Rank'] +
    comparison_df['Error_Rank'] +
    comparison_df['Fidelity_Rank'] +
    comparison_df['Time_Rank']
) / 4

# Sort by overall rank
comparison_df = comparison_df.sort_values('Overall_Rank')
```

```

print("\n" + "="*100)
print("ANSATZ COMPARISON SUMMARY (Averaged across 3 runs)")
print("="*100)
print(comparison_df.to_string())
print("\n" + "="*100)
print("RANKINGS (1 = Best):")
print(" - Lower CNOT count is better (fewer gates)")
print(" - Lower error is better (more accurate)")
print(" - Higher fidelity is better (closer to exact state)")
print(" - Lower time is better (faster convergence)")
print(" - Overall rank is average of all rankings")
print("="*100)

# Save comparison
comparison_df.to_csv("benchmark_comparison_summary.csv")
print(f"\n Comparison summary saved to: benchmark_comparison_summary.csv")

```

```

=====
=====
ANSATZ COMPARISON SUMMARY (Averaged across 3 runs)
=====
=====

          Avg_CNOT  Avg_Depth  Parameters  Conv_Speed_99%  Avg_Time(s)
          Avg_Error(%)  Avg_Fidelity  Avg_Gradient  Plateau_Status  CNOT_Rank  Error_Rank
          Fidelity_Rank  Time_Rank  Overall_Rank

Ansatz
QEB-4q      0.0       3.0        12.0        91.3333    0.2937
0.0000      0.9997      0.0        N/A         2.5        1.5
2.0         1.0       1.750
UCCSD       0.0       16.0        15.0        127.6667   72.4880
0.0000      1.0000      0.0        N/A         2.5        1.5
1.0         4.0       2.250
PC-HEA       0.0       32.0        96.0        300.0000   1.5788
0.1759      0.9969      0.0        N/A         2.5        5.0
5.0         2.0       3.625
UpCCGSD     0.0       37.0        36.0        300.0000   176.2776
0.1714      0.9970      0.0        N/A         2.5        3.5
3.5         5.0       3.625
QEB-8q      176.0      149.0       50.0        300.0000   2.2799
0.1714      0.9970      0.0        N/A         5.0        3.5
3.5         3.0       3.750

=====
=====
RANKINGS (1 = Best):
 - Lower CNOT count is better (fewer gates)
 - Lower error is better (more accurate)

```

- Higher fidelity is better (closer to exact state)
 - Lower time is better (faster convergence)
 - Overall rank is average of all rankings
-
-

Comparison summary saved to: benchmark_comparison_summary.csv

1.9 Step 8: Comprehensive Visualizations

```
[26]: # =====
# STEP 8: COMPARISON PLOTS
# =====

ansatz_names = list(ansatz_dict.keys())
ansatz_names_with_data = results_df['Ansatz'].unique().tolist()
ansatz_names_with_data = [name for name in ansatz_names_with_data if pd.
    ~notna(name)]
print(f"Plotting ansätze: {ansatz_names_with_data}")

# Define specific colors for each ansatz (consistent coloring)
color_map = {
    'UCCSD': '#2E86AB',      # Blue
    'UpCCGSD': '#A23B72',    # Purple
    'PC-HEA': '#F18F01',     # Orange
    'QEB-8q': '#06A77D',    # Green
    'QEB-4q': '#C73E1D'     # Red
}

# Create figure: 1 ROW, 5 COLUMNS
fig, axes = plt.subplots(1, 5, figsize=(28, 6))

# =====
# PLOT 1: Circuit Depth
# =====

ax = axes[0]
for i, ansatz in enumerate(ansatz_names_with_data):
    data = results_df[results_df['Ansatz'] == ansatz]['Circuit_Depth']
    ax.bar(i, data.mean(), yerr=data.std(), color=color_map.get(ansatz, '#999999'),
        alpha=0.7, capsize=5, edgecolor='black', linewidth=1.5)
    ax.set_xticks(range(len(ansatz_names_with_data)))
    ax.set_xticklabels(ansatz_names_with_data, rotation=45, ha='right',
        fontsize=11, fontweight='bold')
    ax.set_ylabel('Circuit Depth', fontsize=13, fontweight='bold')
    ax.set_title('Circuit Depth', fontweight='bold', fontsize=14, pad=10)
    ax.grid(True, alpha=0.3, axis='y', linestyle='--')
```

```

# =====
# PLOT 2: Number of Parameters
# =====
ax = axes[1]
params_data = results_df.groupby('Ansatz')['Num_Parameters'].first()
ax.bar(range(len(params_data)), params_data.values,
       color=[color_map.get(a, '#999999') for a in params_data.index],
       alpha=0.7, edgecolor='black', linewidth=1.5)
ax.set_xticks(range(len(ansatz_names_with_data)))
ax.set_xticklabels(params_data.index, rotation=45, ha='right', fontsize=11, fontweight='bold')
ax.set_ylabel('Number of Parameters', fontsize=13, fontweight='bold')
ax.set_title('Optimization Parameters', fontweight='bold', fontsize=14, pad=10)
ax.grid(True, alpha=0.3, axis='y', linestyle='--')

# =====
# PLOT 3: Energy Error
# =====
ax = axes[2]
for i, ansatz in enumerate(ansatz_names_with_data):
    data = results_df[results_df['Ansatz'] == ansatz]['Energy_Error_Percent']
    # Filter valid data for log scale
    valid_data = data[np.isfinite(data) & (data > 0)]

    if len(valid_data) > 0:
        mean_val = valid_data.mean()
        std_val = valid_data.std()

        ax.bar(i, mean_val, color=color_map.get(ansatz, '#999999'),
               alpha=0.7, edgecolor='black', linewidth=1.5)

        # Add error bar with proper handling for log scale
        if pd.notna(std_val) and std_val > 0:
            # For log scale, use asymmetric error bars
            lower_err = mean_val - max(mean_val * 0.1, mean_val - std_val)
            upper_err = std_val
            ax.errorbar(i, mean_val, yerr=[[lower_err], [upper_err]],
                        fmt='none', ecolor='black', capsize=6, capthick=2,
                        elinewidth=2, alpha=0.7)

    ax.set_xticks(range(len(ansatz_names_with_data)))
    ax.set_xticklabels(ansatz_names_with_data, rotation=45, ha='right', fontsize=11, fontweight='bold')
    ax.set_ylabel('Energy Error (%)', fontsize=13, fontweight='bold')
    ax.set_title('Energy Accuracy', fontweight='bold', fontsize=14, pad=10)
    ax.grid(True, alpha=0.3, axis='y', which='both', linestyle='--')

```

```

ax.set_yscale('log')
# Add chemical accuracy reference
ax.axhline(y=0.16, color='red', linestyle='--', linewidth=2, alpha=0.6,
            label='Chem. Acc.')
ax.legend(fontsize=9, loc='upper left')

# =====
# PLOT 4: Convergence Speed
# =====

ax = axes[3]
for i, ansatz in enumerate(ansatz_names_with_data):
    data = results_df[results_df['Ansatz'] == ansatz]['Convergence_Speed_99']
    # Filter valid data
    valid_data = data[np.isfinite(data) & (data > 0)]

    if len(valid_data) > 0:
        mean_val = valid_data.mean()
        std_val = valid_data.std()

        ax.bar(i, mean_val, color=color_map.get(ansatz, '#999999'),
                alpha=0.7, edgecolor='black', linewidth=1.5)

        if pd.notna(std_val) and std_val > 0:
            ax.errorbar(i, mean_val, yerr=std_val, fmt='none', ecolor='black',
                        capsize=6, capthick=2, elinewidth=2, alpha=0.7)

    ax.set_xticks(range(len(ansatz_names_with_data)))
    ax.set_xticklabels(ansatz_names_with_data, rotation=45, ha='right', u
                      fontsize=11, fontweight='bold')
    ax.set_ylabel('Iterations to 99% Convergence', fontsize=13, fontweight='bold')
    ax.set_title('Convergence Speed', fontweight='bold', fontsize=14, pad=10)
    ax.grid(True, alpha=0.3, axis='y', linestyle='--')

# =====
# PLOT 5: Computation Time
# =====

ax = axes[4]
for i, ansatz in enumerate(ansatz_names_with_data):
    data = results_df[results_df['Ansatz'] == ansatz]['Total_Time_sec']
    # Filter valid data
    valid_data = data[np.isfinite(data) & (data > 0)]

    if len(valid_data) > 0:
        mean_val = valid_data.mean()
        std_val = valid_data.std()

        ax.bar(i, mean_val, color=color_map.get(ansatz, '#999999'),

```

```

        alpha=0.7, edgecolor='black', linewidth=1.5)

    if pd.notna(std_val) and std_val > 0:
        ax.errorbar(i, mean_val, yerr=std_val, fmt='none', ecolor='black',
                    capsize=6, capthick=2, elinewidth=2, alpha=0.7)

ax.set_xticks(range(len(ansatz_names_with_data)))
ax.set_xticklabels(ansatz_names_with_data, rotation=45, ha='right', u
                   ↪fontsize=11, fontweight='bold')
ax.set_ylabel('Time (seconds)', fontsize=13, fontweight='bold')
ax.set_title('Computation Time', fontweight='bold', fontsize=14, pad=10)
ax.grid(True, alpha=0.3, axis='y', linestyle='--')

# Add footnote about QEB-4q if present
if 'QEB-4q' in ansatz_names_with_data:
    fig.text(0.5, 0.02, '* QEB-4q uses different 4-qubit Hamiltonian (not u
                           ↪directly comparable to 8-qubit ansätze)',
              ha='center', fontsize=10, style='italic', color='red', u
              ↪weight='bold')

# Overall title
plt.suptitle(f'LiH VQE Benchmark: Ansatz Comparison u
               ↪({len(ansatz_names_with_data)} Ansätze × {NUM_RUNS} Runs)',
               fontsize=16, fontweight='bold', y=0.98)

plt.tight_layout(rect=[0, 0.04, 1, 0.96])
plt.savefig('benchmark_comparison_plots.png', dpi=150, bbox_inches='tight')
plt.show()

print("Results check:")
for ansatz in ['UCCSD', 'UpCCGSD', 'PC-HEA', 'QEB-8q', 'QEB-4q']:
    data = results_df[results_df['Ansatz'] == ansatz]
    print(f"\n{ansatz}:")
    print(f"  Rows: {len(data)}")
    print(f"  Runs: {data['Run'].unique()}")
    print(f"  Avg Time: {data['Total_Time_sec'].mean():.2f} sec")
    print(f"  Avg Error: {data['Energy_Error_Percent'].mean():.6f}%")
    print(f"  Avg Iters: {data['Total_Iterations'].mean():.0f}")
    print(f"  Circuit Depth: {data['Circuit_Depth'].mean():.0f}")

print("\nConvergence check:")
for ansatz in ['PC-HEA', 'QEB-8q', 'QEB-4q']:
    data = results_df[results_df['Ansatz'] == ansatz].iloc[0]
    conv_hist = data.get('_convergence_history', [])
    print(f"{ansatz}: {len(conv_hist)} evaluations")
    if len(conv_hist) > 0:

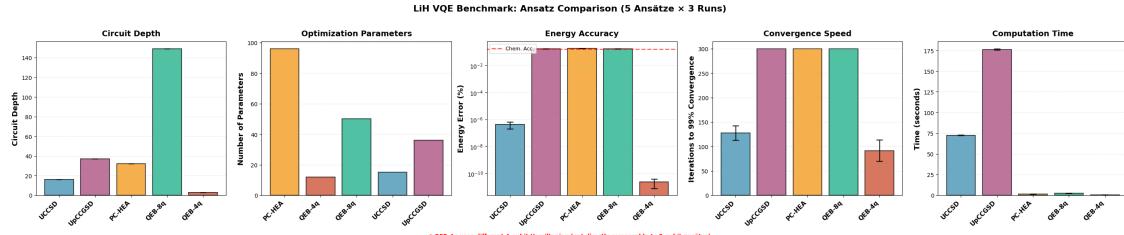
```

```

print(f" Initial: {conv_hist[0]:.6f} Ha")
print(f" Final: {conv_hist[-1]:.6f} Ha")

```

Plotting ansätze: ['UCCSD', 'UpCCGSD', 'PC-HEA', 'QEB-8q', 'QEB-4q']



Results check:

UCCSD:

Rows: 3
Runs: [1. 2. 3.]
Avg Time: 72.49 sec
Avg Error: 0.000000%
Avg Iters: 300
Circuit Depth: 16

UpCCGSD:

Rows: 3
Runs: [1. 2. 3.]
Avg Time: 176.28 sec
Avg Error: 0.171354%
Avg Iters: 300
Circuit Depth: 37

PC-HEA:

Rows: 3
Runs: [1. 2. 3.]
Avg Time: 1.58 sec
Avg Error: 0.175857%
Avg Iters: 300
Circuit Depth: 32

QEB-8q:

Rows: 3
Runs: [1. 2. 3.]
Avg Time: 2.28 sec
Avg Error: 0.171372%
Avg Iters: 300
Circuit Depth: 149

```

QEB-4q:
  Rows: 3
  Runs: [1. 2. 3.]
  Avg Time: 0.29 sec
  Avg Error: 0.000000%
  Avg Iters: 265
  Circuit Depth: 3

```

```

Convergence check:
PC-HEA: 0 evaluations
QEB-8q: 0 evaluations
QEB-4q: 0 evaluations

```

```

[27]: # =====
# STEP 8: COMPARISON PLOTS
# =====

ansatz_names = list(ansatz_dict.keys())
ansatz_names_with_data = results_df['Ansatz'].unique().tolist()
ansatz_names_with_data = [name for name in ansatz_names_with_data if pd.
    ~notna(name)]
print(f"Plotting ansätze: {ansatz_names_with_data}")

# Define specific colors for each ansatz (consistent coloring)
color_map = {
    'UCCSD': '#2E86AB',      # Blue
    'UpCCGSD': '#A23B72',    # Purple
    'PC-HEA': '#F18F01',     # Orange
    'QEB-8q': '#06A77D',    # Green
    'QEB-4q': '#C73E1D'     # Red
}

# Create figure: 1 ROW, 5 COLUMNS
fig, axes = plt.subplots(1, 5, figsize=(28, 6))

# =====
# PLOT 1: Circuit Depth
# =====

ax = axes[0]
for i, ansatz in enumerate(ansatz_names_with_data):
    data = results_df[results_df['Ansatz'] == ansatz]['Circuit_Depth']
    ax.bar(i, data.mean(), yerr=data.std(), color=color_map.get(ansatz, '#999999'),
            alpha=0.7, capsize=5, edgecolor='black', linewidth=1.5)
ax.set_xticks(range(len(ansatz_names_with_data)))

```

```

ax.set_xticklabels(ansatz_names_with_data, rotation=45, ha='right', u
    ↪fontsize=11, fontweight='bold')
ax.set_ylabel('Circuit Depth', fontsize=13, fontweight='bold')
ax.set_title('Circuit Depth', fontweight='bold', fontsize=14, pad=10)
ax.grid(True, alpha=0.3, axis='y', linestyle='--')

# =====
# PLOT 2: Number of Parameters
# =====
ax = axes[1]
params_data = results_df.groupby('Ansatz')['Num_Parameters'].first()
ax.bar(range(len(params_data)), params_data.values,
       color=[color_map.get(a, '#999999') for a in params_data.index],
       alpha=0.7, edgecolor='black', linewidth=1.5)
ax.set_xticks(range(len(ansatz_names_with_data)))
ax.set_xticklabels(params_data.index, rotation=45, ha='right', fontsize=11, u
    ↪fontweight='bold')
ax.set_ylabel('Number of Parameters', fontsize=13, fontweight='bold')
ax.set_title('Optimization Parameters', fontweight='bold', fontsize=14, pad=10)
ax.grid(True, alpha=0.3, axis='y', linestyle='--')

# =====
# PLOT 3: Energy Error
# =====
ax = axes[2]
for i, ansatz in enumerate(ansatz_names_with_data):
    data = results_df[results_df['Ansatz'] == ansatz]['Energy_Error_Percent']
    # Filter valid data for log scale
    valid_data = data[np.isfinite(data) & (data > 0)]

    if len(valid_data) > 0:
        mean_val = valid_data.mean()
        std_val = valid_data.std()

        ax.bar(i, mean_val, color=color_map.get(ansatz, '#999999'),
               alpha=0.7, edgecolor='black', linewidth=1.5)

        # Add error bar with proper handling for log scale
        if pd.notna(std_val) and std_val > 0:
            # For log scale, use asymmetric error bars
            lower_err = mean_val - max(mean_val * 0.1, mean_val - std_val)
            upper_err = std_val
            ax.errorbar(i, mean_val, yerr=[[lower_err], [upper_err]],
                        fmt='none', ecolor='black', capsize=6, capthick=2,
                        elinewidth=2, alpha=0.7)

    ax.set_xticks(range(len(ansatz_names_with_data)))

```

```

ax.set_xticklabels(ansatz_names_with_data, rotation=45, ha='right', u
    ↪fontsize=11, fontweight='bold')
ax.set_ylabel('Energy Error (%)', fontsize=13, fontweight='bold')
ax.set_title('Energy Accuracy', fontweight='bold', fontsize=14, pad=10)
ax.grid(True, alpha=0.3, axis='y', which='both', linestyle='--')
ax.set_yscale('log')
# Add chemical accuracy reference
ax.axhline(y=0.16, color='red', linestyle='--', linewidth=2, alpha=0.6,
            label='Chem. Acc.')
ax.legend(fontsize=9, loc='upper left')

# =====
# PLOT 4: Convergence Speed
# =====
ax = axes[3]
for i, ansatz in enumerate(ansatz_names_with_data):
    data = results_df[results_df['Ansatz'] == ansatz]['Convergence_Speed_99']
    # Filter valid data
    valid_data = data[np.isfinite(data) & (data > 0)]

    if len(valid_data) > 0:
        mean_val = valid_data.mean()
        std_val = valid_data.std()

        ax.bar(i, mean_val, color=color_map.get(ansatz, '#999999'),
                alpha=0.7, edgecolor='black', linewidth=1.5)

        if pd.notna(std_val) and std_val > 0:
            ax.errorbar(i, mean_val, yerr=std_val, fmt='none', ecolor='black',
                        capsize=6, capthick=2, elinewidth=2, alpha=0.7)

ax.set_xticks(range(len(ansatz_names_with_data)))
ax.set_xticklabels(ansatz_names_with_data, rotation=45, ha='right', u
    ↪fontsize=11, fontweight='bold')
ax.set_ylabel('Iterations to 99% Convergence', fontsize=13, fontweight='bold')
ax.set_title('Convergence Speed', fontweight='bold', fontsize=14, pad=10)
ax.grid(True, alpha=0.3, axis='y', linestyle='--')

# =====
# PLOT 5: Computation Time
# =====
ax = axes[4]
for i, ansatz in enumerate(ansatz_names_with_data):
    data = results_df[results_df['Ansatz'] == ansatz]['Total_Time_sec']
    # Filter valid data
    valid_data = data[np.isfinite(data) & (data > 0)]

```

```

if len(valid_data) > 0:
    mean_val = valid_data.mean()
    std_val = valid_data.std()

    ax.bar(i, mean_val, color=color_map.get(ansatz, '#999999'),
           alpha=0.7, edgecolor='black', linewidth=1.5)

    if pd.notna(std_val) and std_val > 0:
        ax.errorbar(i, mean_val, yerr=std_val, fmt='none', ecolor='black',
                     capsize=6, capthick=2, elinewidth=2, alpha=0.7)

ax.set_xticks(range(len(ansatz_names_with_data)))
ax.set_xticklabels(ansatz_names_with_data, rotation=45, ha='right', fontweight='bold')
ax.set_ylabel('Time (seconds)', fontsize=13, fontweight='bold')
ax.set_title('Computation Time', fontweight='bold', fontsize=14, pad=10)
ax.grid(True, alpha=0.3, axis='y', linestyle='--')

# Add footnote about QEB-4q if present
if 'QEB-4q' in ansatz_names_with_data:
    fig.text(0.5, 0.02, '* QEB-4q uses different 4-qubit Hamiltonian (not directly comparable to 8-qubit ansätze)', ha='center', fontsize=10, style='italic', color='red', weight='bold')

# Overall title
plt.suptitle(f'LiH VQE Benchmark: Ansatz Comparison\n({len(ansatz_names_with_data)} Ansätze × {NUM_RUNS} Runs)', fontsize=16, fontweight='bold', y=0.98)

plt.tight_layout(rect=[0, 0.04, 1, 0.96])
plt.savefig('benchmark_comparison_plots.png', dpi=150, bbox_inches='tight')
plt.show()

print("Results check:")
for ansatz in ['UCCSD', 'UpCCGSD', 'PC-HEA', 'QEB-8q', 'QEB-4q']:
    data = results_df[results_df['Ansatz'] == ansatz]
    print(f"\n{ansatz}:")
    print(f"  Rows: {len(data)}")
    print(f"  Runs: {data['Run'].unique()}")
    print(f"  Avg Time: {data['Total_Time_sec'].mean():.2f} sec")
    print(f"  Avg Error: {data['Energy_Error_Percent'].mean():.6f}%")
    print(f"  Avg Iters: {data['Total_Iterations'].mean():.0f}")
    print(f"  Circuit Depth: {data['Circuit_Depth'].mean():.0f}")

print("\nConvergence check:")

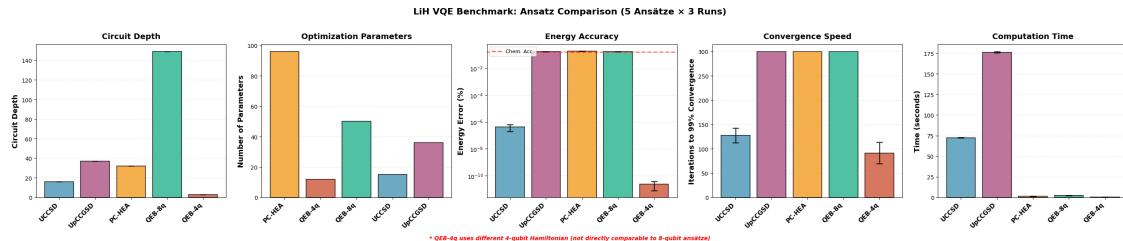
```

```

for ansatz in ['PC-HEA', 'QEB-8q', 'QEB-4q']:
    data = results_df[results_df['Ansatz'] == ansatz].iloc[0]
    conv_hist = data.get('_convergence_history', [])
    print(f"{ansatz}: {len(conv_hist)} evaluations")
    if len(conv_hist) > 0:
        print(f"  Initial: {conv_hist[0]:.6f} Ha")
        print(f"  Final: {conv_hist[-1]:.6f} Ha")

```

Plotting ansätze: ['UCCSD', 'UpCCGSD', 'PC-HEA', 'QEB-8q', 'QEB-4q']



Results check:

UCCSD:

Rows: 3
Runs: [1. 2. 3.]
Avg Time: 72.49 sec
Avg Error: 0.000000%
Avg Iters: 300
Circuit Depth: 16

UpCCGSD:

Rows: 3
Runs: [1. 2. 3.]
Avg Time: 176.28 sec
Avg Error: 0.171354%
Avg Iters: 300
Circuit Depth: 37

PC-HEA:

Rows: 3
Runs: [1. 2. 3.]
Avg Time: 1.58 sec
Avg Error: 0.175857%
Avg Iters: 300
Circuit Depth: 32

QEB-8q:

Rows: 3

```

Runs: [1. 2. 3.]
Avg Time: 2.28 sec
Avg Error: 0.171372%
Avg Iters: 300
Circuit Depth: 149

```

```

QEB-4q:
Rows: 3
Runs: [1. 2. 3.]
Avg Time: 0.29 sec
Avg Error: 0.000000%
Avg Iters: 265
Circuit Depth: 3

```

```

Convergence check:
PC-HEA: 0 evaluations
QEB-8q: 0 evaluations
QEB-4q: 0 evaluations

```

```

[28]: # =====
# All-Ansatz Convergence Comparison (Best-So-Far)
# =====

print("\n" + "="*70)
print("CREATING UNIFIED CONVERGENCE COMPARISON PLOT")
print("="*70)

# Define all 5 ansätze for this unified plot
ansatz_names_all = ['UCCSD', 'UpCCGSD', 'PC-HEA', 'QEB-8q', 'QEB-4q']

# Create a comprehensive comparison plot showing all 5 ansätze
# Changed to taller figure with square-ish subplots
fig = plt.figure(figsize=(16, 64)) # Even taller for 4 subplots
gs = fig.add_gridspec(4, 1, hspace=0.25)

colors = {
    'UCCSD': '#1f77b4',
    'UpCCGSD': '#ff7f0e',
    'PC-HEA': '#2ca02c',
    'QEB-8q': '#9467bd', # Purple for 8q QEB
    'QEB-4q': '#d62728' # Red for 4q QEB (same as 'QEB' in final-1)
}

markers = {
    'UCCSD': 'o',
    'UpCCGSD': 's',
    'PC-HEA': '^',
}

```

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        'QEB-8q': 'D',
        'QEB-4q': 'v'
    }

# Plot 1: Energy Convergence (Best-So-Far) with Dual Y-Axis
ax1 = fig.add_subplot(gs[0, 0])
ax1.set_title('Energy Convergence: All 5 Ansätze (Best-So-Far)', fontsize=20,
              fontweight='bold', pad=20)

# Collect all 8q data to determine range (including QEB-8q now)
all_8q_energies = []
for ansatz_name in ['UCCSD', 'UpCCGSD', 'PC-HEA', 'QEB-8q']:
    ansatz_results = [r for r in all_results if isinstance(r, dict) and
                      r.get('Ansatz') == ansatz_name and r.get('Run') == 2]
    if not ansatz_results:
        continue
    result = ansatz_results[0]
    conv_hist = result.get('_convergence_history', [])
    all_8q_energies.extend(conv_hist)
    iterations = range(1, len(conv_hist) + 1)
    ax1.plot(iterations, conv_hist, color=colors[ansatz_name],
              linewidth=3.5, label=f"{ansatz_name} (8q)", alpha=0.85)

ax1.axhline(y=exact_electronic, color='black', linestyle='--', linewidth=3,
             alpha=0.7, label='Exact (8q)')
all_8q_energies.append(exact_electronic)

# Add text annotation for 8q exact energy
ax1.text(0.02, 0.02, f'8q Exact: {exact_electronic:.6f} Ha',
         transform=ax1.transAxes, fontsize=15, verticalalignment='bottom',
         bbox=dict(boxstyle='round', facecolor='wheat', alpha=0.8))

ax1.set_xlabel('Evaluation Number', fontsize=17, labelpad=10)
ax1.set_ylabel('Electronic Energy (Ha) - 8 qubits', fontsize=17, color='black',
               labelpad=10)
# Add 10% padding to the range
energy_range_8q = max(all_8q_energies) - min(all_8q_energies)
padding_8q = energy_range_8q * 0.10
ax1.set_ylim(min(all_8q_energies) - padding_8q, max(all_8q_energies) +
             padding_8q)
ax1.tick_params(axis='y', labelcolor='black', labelsize=15)
ax1.tick_params(axis='x', labelsize=15)
ax1.grid(True, alpha=0.4, linestyle=':', linewidth=1.2)

# Create secondary y-axis for QEB-4q
ax1_right = ax1.twinx()
# Get the LONGEST QEB-4q run (300 iterations from final benchmark)

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qeb_results = [r for r in all_results if isinstance(r, dict) and
               r.get('Ansatz') == 'QEB-4q' and r.get('Run') == 2]
if qeb_results:
    # Find the run with most iterations
    result = max(qeb_results, key=lambda r: r.get('Total_Iterations', 0))
    conv_hist = result.get('_convergence_history', [])
    iterations = range(1, len(conv_hist) + 1)
    ax1_right.plot(iterations, conv_hist, color=colors['QEB-4q'],
                    linewidth=3.5, label=f"QEB-4q (4q)", alpha=0.85)

    exact_4q = result['Exact_Energy_Ha']
    ax1_right.axhline(y=exact_4q, color='darkred', linestyle=':',
                        linewidth=3, alpha=0.7, label='Exact (4q)')

    # Add text annotation for 4q exact energy
    ax1_right.text(0.98, 0.02, f'4q Exact: {exact_4q:.6f} Ha',
                   transform=ax1.transAxes, fontsize=15,
                   verticalalignment='bottom',
                   horizontalalignment='right',
                   bbox=dict(boxstyle='round', facecolor='lightcoral', alpha=0.8))

    ax1_right.set_ylabel('Electronic Energy (Ha) - 4 qubits', fontsize=17,
                         color=colors['QEB-4q'], labelpad=10)
    ax1_right.tick_params(axis='y', labelcolor=colors['QEB-4q'], labelsize=15)
    # Add 10% padding to QEB range
    all_4q_energies = conv_hist + [exact_4q]
    energy_range_4q = max(all_4q_energies) - min(all_4q_energies)
    padding_4q = energy_range_4q * 0.10
    ax1_right.set_ylim(min(all_4q_energies) - padding_4q, max(all_4q_energies) +
                       padding_4q)

    # Combine legends
    lines1, labels1 = ax1.get_legend_handles_labels()
    lines2, labels2 = ax1_right.get_legend_handles_labels()
    ax1.legend(lines1 + lines2, labels1 + labels2, fontsize=14, loc='upper right')

    # Plot 2: Absolute Error (Log Scale)
    ax2 = fig.add_subplot(gs[1, 0])
    ax2.set_title('Absolute Energy Error: Run 2 Comparison (Log Scale)',
                  fontsize=20, fontweight='bold', pad=20)

    # Collect all error data to determine range
    all_errors = []
    for ansatz_name in ansatz_names_all:
        ansatz_results = [r for r in all_results if isinstance(r, dict) and
                          r.get('Ansatz') == ansatz_name and r['Run'] == 2]

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if not ansatz_results:
    continue

# Get the longest run
result = max(ansatz_results, key=lambda r: r.get('Total_Iterations', 0))

conv_hist = result.get('_convergence_history', [])
exact = result['Exact_Energy_Ha']
errors = [abs(e - exact) for e in conv_hist]
all_errors.extend(errors)
iterations = range(1, len(errors) + 1)
ax2.semilogy(iterations, errors, color=colors[ansatz_name],
              linewidth=3.5, label=ansatz_name, marker=markers[ansatz_name],
              markevery=max(1, len(errors)//15), markersize=9, alpha=0.85)

ax2.set_xlabel('Evaluation Number', fontsize=17, labelpad=10)
ax2.set_ylabel('Absolute Error (Ha) - Log Scale', fontsize=17, labelpad=10)
ax2.legend(fontsize=14, loc='upper right')
ax2.grid(True, alpha=0.4, which='both', linestyle=':', linewidth=1.2)
# Set range with padding - use powers of 10 for log scale
min_error = min([e for e in all_errors if e > 0]) # Avoid log(0)
max_error = max(all_errors)
# Go down one order of magnitude below min, up one above max
ax2.set_ylim(10**(np.floor(np.log10(min_error)) - 0.5),
             10**(np.ceil(np.log10(max_error)) + 0.5))
ax2.tick_params(labelsize=15)

# Plot 3: Energy Error Percentage (Linear Scale)
ax3 = fig.add_subplot(gs[2, 0])
ax3.set_title('Energy Error Percentage: Run 2 Comparison',
              fontsize=20, fontweight='bold', pad=20)

# Collect all percentage error data
all_errors_pct = []
for ansatz_name in ansatz_names_all:
    ansatz_results = [r for r in all_results if isinstance(r, dict) and
                      r.get('Ansatz') == ansatz_name and r['Run'] == 2]
    if not ansatz_results:
        continue

    # Get the longest run
    result = max(ansatz_results, key=lambda r: r.get('Total_Iterations', 0))

    conv_hist = result.get('_convergence_history', [])
    exact = result['Exact_Energy_Ha']
    # Calculate percentage error
    errors_pct = [(abs(e - exact) / abs(exact)) * 100 for e in conv_hist]

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all_errors_pct.extend(errors_pct)
iterations = range(1, len(errors_pct) + 1)
ax3.plot(iterations, errors_pct, color=colors[ansatz_name],
          linewidth=3.5, label=ansatz_name, marker=markers[ansatz_name],
          markevery=max(1, len(errors_pct)//15), markersize=9, alpha=0.85)

ax3.set_xlabel('Evaluation Number', fontsize=17, labelpad=10)
ax3.set_ylabel('Energy Error (%)', fontsize=17, labelpad=10)
ax3.legend(fontsize=14, loc='upper right')
ax3.grid(True, alpha=0.4, linestyle=':', linewidth=1.2)
ax3.tick_params(labelsize=15)

# Much more aggressive padding for Graph 3
min_pct = min(all_errors_pct)
max_pct = max(all_errors_pct)
range_pct = max_pct - min_pct

# Use 25% relative padding OR at least 0.02% absolute padding
relative_padding = range_pct * 0.25
abs_padding = 0.02 # 0.02% minimum padding
padding_pct = max(relative_padding, abs_padding)

# Set limits with guaranteed space at bottom
y_min = max(0, min_pct - padding_pct)
y_max = max_pct + padding_pct

# If y_min is still very close to 0, add a bit more
if y_min < 0.01:
    y_min = -0.01 # Small negative value to ensure visible space

ax3.set_ylim(y_min, y_max)

# Plot 4: Final Energy Error Bar Chart - ALL RUNS
ax4 = fig.add_subplot(gs[3, 0])
ax4.set_title('Final Energy Errors: All Runs',
              fontsize=20, fontweight='bold', pad=20)

# Collect final errors for each ansatz across all runs
run_colors = {1: '#6baed6', 2: '#fd8d3c', 3: '#74c476'} # Blue, Orange, Green
bar_width = 0.17 # Narrower bars for 5 ansätze
x_positions = np.arange(len(ansatz_names_all))

# For each run, collect final errors
for run_idx in [1, 2, 3]:
    errors_for_run = []
    for ansatz_name in ansatz_names_all:
        ansatz_results = [r for r in all_results if isinstance(r, dict) and

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        r.get('Ansatz') == ansatz_name and r.get('Run') == run_idx]
    if not ansatz_results:
        errors_for_run.append(0)
        continue

    # Get the longest run for this specific run number
    result = max(ansatz_results, key=lambda r: r.get('Total Iterations', 0))

    conv_hist = result.get('_convergence_history', [])
    if conv_hist:
        final_energy = conv_hist[-1]
        exact = result['Exact_Energy_Ha']
        final_error = abs(final_energy - exact)
        errors_for_run.append(final_error)
    else:
        errors_for_run.append(0)

    # Plot bars for this run
    offset = (run_idx - 2) * bar_width # -1, 0, +1 for runs 1, 2, 3
    ax4.bar(x_positions + offset, errors_for_run, bar_width,
            label=f'Run {run_idx}', color=run_colors[run_idx],
            alpha=0.8, edgecolor='black', linewidth=1.5)

    ax4.set_xlabel('Ansatz', fontsize=17, labelpad=10)
    ax4.set_ylabel('Absolute Error (Ha)', fontsize=17, labelpad=10)
    ax4.set_xticks(x_positions)
    ax4.set_xticklabels(ansatz_names_all, fontsize=15)
    ax4.tick_params(axis='y', labelsize=15)
    ax4.legend(fontsize=14, loc='upper right')
    ax4.grid(True, alpha=0.4, axis='y', linestyle=':', linewidth=1.2)
    ax4.set_yscale('log') # Use log scale like in the reference image

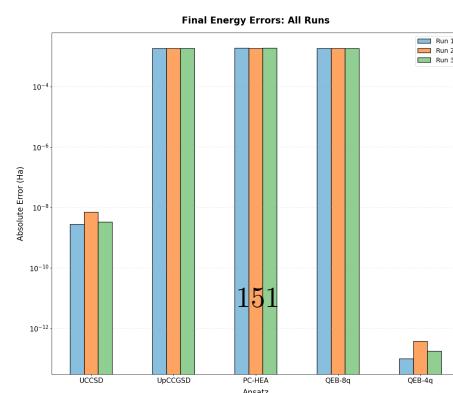
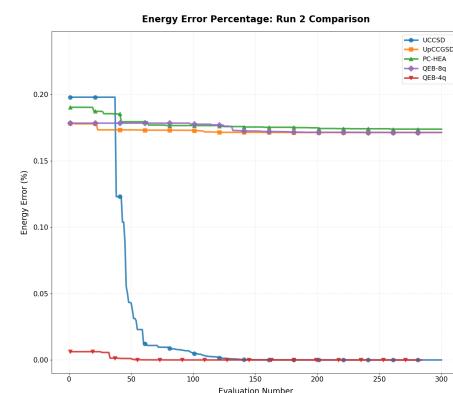
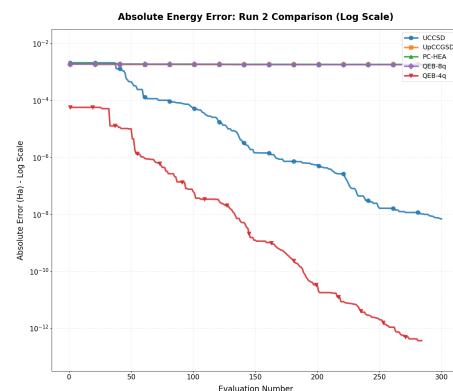
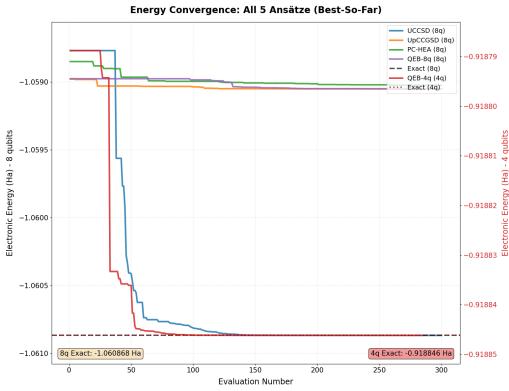
    plt.suptitle('LiH VQE Benchmark: All-Ansatz Comparison (5 Ansätze, Run 2)',
                 fontsize=22, fontweight='bold', y=0.9985)
    plt.savefig('all_5_ansatz_convergence_comparison.png', dpi=150,
                bbox_inches='tight')
    plt.show()

print("\n Comprehensive convergence comparison plot saved!")
print(" File: all_5_ansatz_convergence_comparison.png")
print(f" Ansätze plotted: {ansatz_names_all}")

```

=====
CREATING UNIFIED CONVERGENCE COMPARISON PLOT
=====

LiH VQE Benchmark: All-Ansatz Comparison (5 Ansätze, Run 2)



Comprehensive convergence comparison plot saved!
File: all_5_ansatz_convergence_comparison.png
Ansätze plotted: ['UCCSD', 'UpCCGSD', 'PC-HEA', 'QEB-8q', 'QEB-4q']