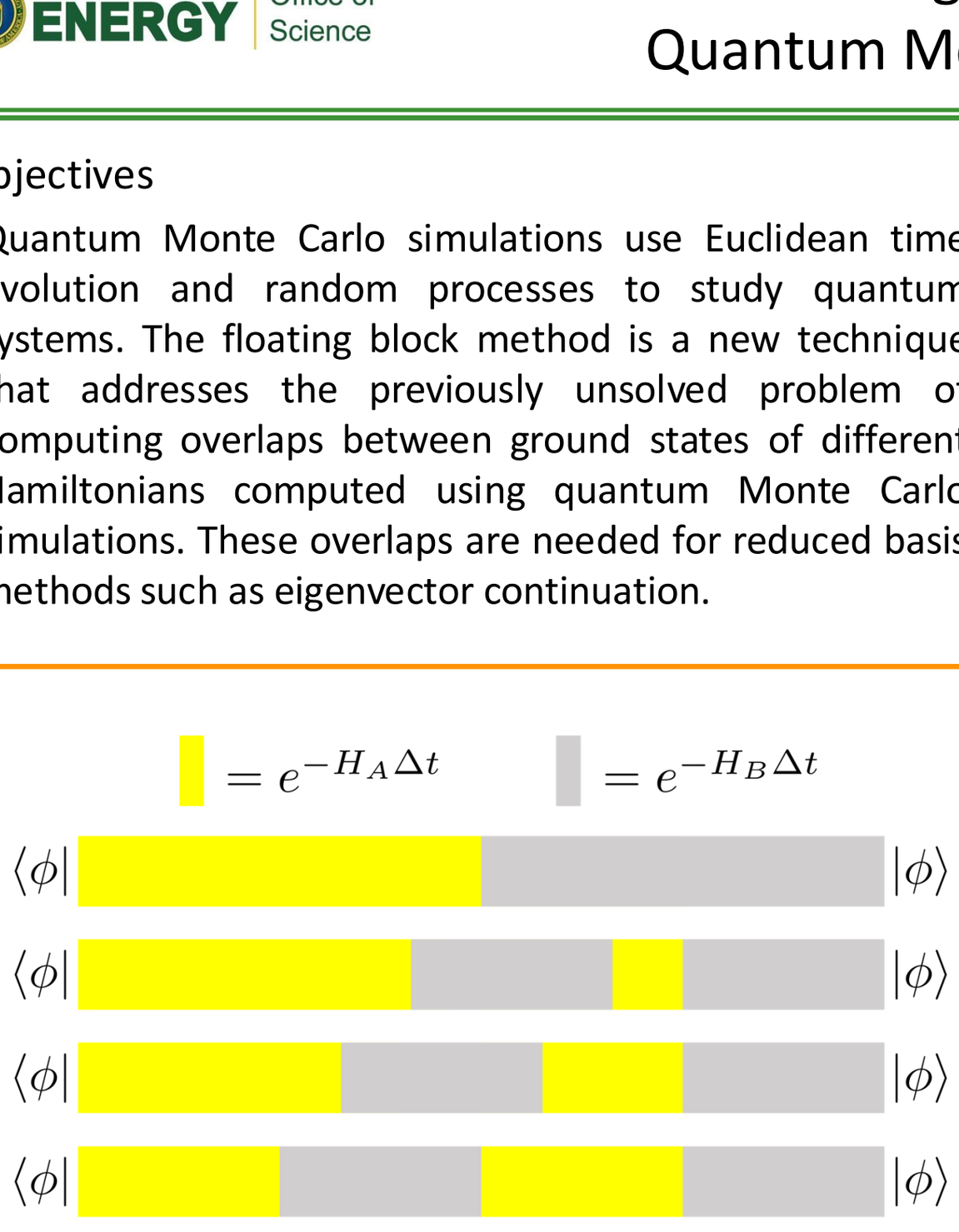
Floating Block Method for Quantum Monte Carlo Simulations

Objectives

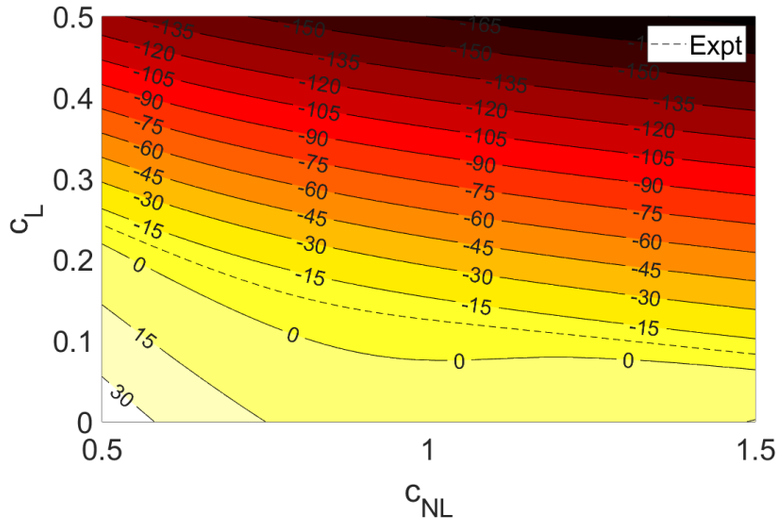
- Quantum Monte Carlo simulations use Euclidean time evolution and random processes to study quantum systems. The floating block method is a new technique that addresses the previously unsolved problem of computing overlaps between ground states of different Hamiltonians computed using quantum Monte Carlo simulations. These overlaps are needed for reduced basis methods such as eigenvector continuation.



Schematic diagram showing the Euclidean time evolution corresponding to two different Hamiltonians, H_A and H_B. In the limit of large Euclidean time, the ratio between the bottom-row amplitude and the top-row amplitude gives the overlap probability between the normalized ground states of H_A and H_B.

Impact (as of now)

- With the floating block method, eigenvector continuation can now be performed using quantum Monte Carlo simulations. The figure below shows the difference between the emulated energy for ^{12}C and the triple-α threshold. c_L is the coefficient of the local two nucleon interaction, and c_{NL} is the coefficient of the nonlocal two-nucleon interaction. The dashed line shows the contour for the observed experimental value.



Accomplishments (as of now)

- "Floating Block Method for Quantum Monte Carlo Simulations", Sarkar, Lee, Meißner, Phys. Rev. Lett. 131, 242503 (2023)
- DOE Highlight