NUCLEI
Nuclear Computational Low-Energy Initiative

U.S. DEPARTMENT OF ENERGY | Office of Science

Quantum Monte Carlo Calculations for Nuclear Physics

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Quantum Monte Carlo

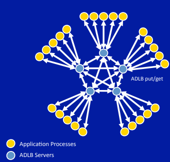
Physics Problem: Determine the structure of nuclei, including ground state and spectrum of excited states, electromagnetic form factors and transition rates. Theory versus experiment: In many cases, the experimental results are known, but theory has suggested new which have then been observed.

Computational approach: Use Monte Carlo methods to predict the results of the many-nucleon Schrödinger equation for realistic 2- and 3-nucleon interactions. The strong nucleon spin and orbital angular momentum correlations present in the interactions must be accounted for.

Advantages: Monte Carlo does not require a basis expansion or fixed grids

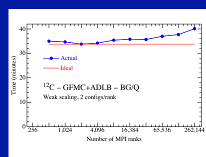
Difficulties: Keeping track of every nucleon's spin and isospin states: the number of spin states is $2^A \binom{A}{Z}$, where A = # nucleons and Z = # protons. In Green's function Monte Carlo (GFMC) these states are summed explicitly, while in Auxiliary Field Diffusion Monte Carlo (AFDMC) they are sampled using Monte Carlo methods. GFMC is more appropriate for Light Nuclei, AFDMC for heavy nuclei and matter.

Highly Parallel Green's Function Monte Carlo for Nuclear Physics

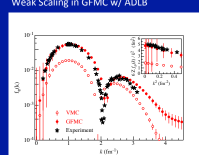


GFMC uses all the nucleon spin and isospin states and thus the computational cost increases rapidly with the number of nucleons.

- At beginning of SciDAC, GFMC was computing all of the above for A = 10 (beryllium, boron) with a parallel manager/worker algorithm with load balancing (2000 MPI processes on IBM SP at NERSC).
  - The computation depended on doing several (>10) Monte Carlo samples per process.
- Computational challenge: Wanted to do ^{12}C, an important nucleus, which was within range with ~100,000 processes.
  - Needed to use more processes than Monte Carlo samples, so had to break one sample across multiple processes, leading to much finer grain parallelism, and more complex task scheduling and load balancing
  - Wanted to maintain overall manager/worker structure



Weak Scaling in GFMC w/ ADLB



Transition form factor for decay of the ^{12}C Hoyle state to the ground state. The GFMC result is in excellent agreement with experiment.

Computer Science response via SciDAC: The Asynchronous Dynamic Load Balancing library (ADLB)

- ADLB is a library that implements a flexible and scalable scheduling and load-balancing system for work units of varying types, sizes, and priorities.
  - There is no manager process; rather, a subset of application processes in constant communication with one another is used to manage in the background a shared pool of work units.
  - Application processes create and *put* work units into this pool and *get* and process work units from this pool.
  - Sophisticated (i.e. complicated) process-load balancing, memory-usage load balancing, and message-traffic load balancing algorithms are used to achieve scalability without burdening the application programmer.
  - ADLB uses MPI and is also compatible with other MPI usage by the application.
  - Work units can create sub-work units for ADLB to assign to other processors and return the results.
  - Work units can be parallelized with OpenMP.
- Physics Results enabled: We were able to carry out the desired computations for ^{12}C, including Hoyle state and its decay rate to the ground state, with excellent scaling on BG/P.
- Current and future work:
  - More demanding computations: response functions for ^{12}C on BG/Q
  - Required: larger work packages, providing memory management challenges
  - Solution: new distributed memory management library (DMEM) in addition to ADLB
    - API summary: put, get, copy, free, get-part, update
    - User (application or another library) refers to a memory object via a (small) *handle*, which encodes its location and size.
    - DMEM manages memory on all clients. Runs as separate thread, sharing memory with application processes, so local operations are fast.
    - Optimization: put and copy operations are local if possible.
    - ADLB is then free to manage only DMEM handles, which are tiny, thus reducing requirement for lots of servers just for memory reasons.
    - Looking ahead, size is of type MPI_Aint, which is typically a long int in C and an integer*8 in Fortran, thus supporting large work packages.
  - VLMPI: MPI extension for > 2GB messages
    - will be used by DMEM, thus providing large work packages for ADLB
    - Usable by other applications

The ADLB API: a Simple Programming Model

- Basic calls
  - ADLB_Init(num_servers, am_server, app_comm)
  - ADLB_Server()
  - ADLB_Put(type, priority, len, buf, target_rank, answer_dest)
  - ADLB_Reserve(req_types, handle, len, type, prio, answer_dest)
  - ADLB_Ireserve(…)
  - ADLB_Get_Reserved(handle, buffer)
  - ADLB_Set_Done()
  - ADLB_Finalize()
- Types, answer_rank, target_rank can be used to implement some common patterns
  - Sending a message
  - Decomposing a task into subtasks
  - Dependencies among tasks are dynamic and implemented via types & priorities

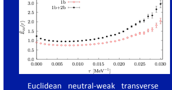
Electron and Neutrino Scattering from ^4He and ^{12}C

Objectives

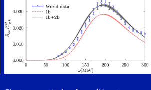
- Compute the electron scattering of ^4He and ^{12}C for which accurate experimental data are available.
- Within the same formalism, study the neutral-current and charged-current response functions, fundamental ingredients for describing neutrino-^{12}C scattering.
- Investigate the energy dependence of the two-body meson-exchange currents contributions.

Impact

- The calculations of the Euclidean electromagnetic response function of ^{12}C can be used to predict the results of the latest electron-^{12}C scattering experiment of JLab.
- Accurate calculations of electroweak response functions are relevant to neutrino-nucleus scattering experiment (e.g. MiniBoone). Further work on charged-current scattering is planned.



Euclidean neutral-weak transverse response functions of ^{12}C at q = 570 MeV. Two-body currents increase the one-body response in both the quasielastic and threshold regions.



Electron scattering from ^4He at q = 600 MeV obtained from the corresponding Euclidean response by using Maximum Entropy techniques.

Accomplishments

- Development of an algorithm to compute the Euclidean response functions within Green's function Monte Carlo.
- Using Maximum Entropy techniques it is now possible to obtain the electromagnetic response of ^4He from the Euclidean response.
- Two-body currents and nuclear correlations have to be accounted for in order to get good agreement with experimental data.

Hyperons in Neutron Stars(?): Hyperon-Neutron-Neutron Interactions

Objectives

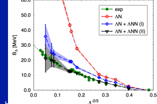
- Study the ground state properties of Λ-hypernuclei over a wide mass range (3 ≤ A ≤ 91).
- Investigate the effect of the presence of hyperons in the inner core of neutron stars.

Impact

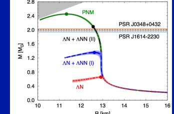
- Extension of ab-initio calculations to the strange nuclear sector.
- Provide the directions for future theoretical investigation and for the next generation of terrestrial hypernuclear experiments.
- New hints for the solution of the so-called *hyperon puzzle*: connection between the theory of baryon-baryon interaction and the mass-radius relation in neutron stars.

Accomplishments

- Development of quantum Monte Carlo methods to explore nuclear systems with hyperons.
- Improvement of existing realistic hyperon-nucleon Hamiltonians.
- Point out the need of additional hypernuclear experimental input and further theoretical studies.



Hyperon separation energy. The inclusion of three-body hyperon-nucleon forces provides a good description of the ground state physics of Λ-hypernuclei over a wide mass range.



Mass radius relation. Different models of three-body hyperon-nucleon force predict dramatically different results on the maximum mass of neutron stars.

Magnetic Moments and Transitions in Light Nuclei

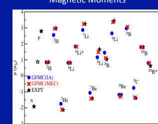
Objectives:

- Understand electromagnetic properties and transition rates of light nuclei
- Test realistic interactions and currents, including complete two-nucleon currents

Impact:

- Much improved description of all moments and electromagnetic transitions
- Increased confidence in our ability to explain electron and neutrino scattering from nuclei

Magnetic Moments

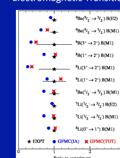


Accomplishments

Green's Function Monte Carlo (GFMC) calculations of light nuclei give accurate energies but a lowest-order theory of one-body currents (blue) disagrees with experiment (black).

Including two-nucleon currents based on effective field theory (red) improves all predictions!

Electromagnetic Transitions



Single-, Two-Nucleon and Cluster Momentum Distributions in A ≤ 12 Nuclei

Objectives:

- Calculate single-, two-nucleon and cluster momentum distributions in nuclei
- These momentum distributions are probed in back-to-back experiments at JLAB, BNL, and Fermilab, including the relative abundance of np vs pp pairs.

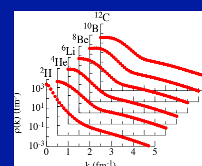
Accomplishments

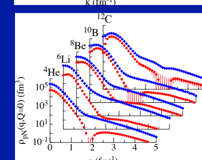
- We have calculated these momentum distributions in light nuclei up to Carbon (A=12)
- Two-nucleon momentum distributions have been evaluated for 8 nuclear states in pair ST and *pp*, *pn*, *nn* projections, as functions of relative momentum *q* and total momentum *Q*; the large ratio of *pn* to *pp* pairs observed in (*e,e'pN*) experiments is easily understood due to strong tensor force between *pn* pairs.

Impact

of the abundance of np (vs pp or nn) pairs is understood as arising from the tensor NN interaction, which is important in relative s-waves.

- All these results are posted on-line as figures and tables, along with various cluster distributions like *dp*, *tp*, *αd*. (www.phy.anl.gov/theory/research/momenta)





Larger Nuclei and Neutron-Rich Matter: Auxiliary Field Diffusion Monte Carlo

Objectives:

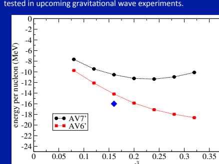
- Calculate heavier nuclei, including neutron-rich nuclei important in the r-process, using realistic NN and NNN interactions.
- Auxiliary Field Diffusion Monte Carlo methods sample the spins and isospins using Monte Carlo methods in addition to the spatial coordinates. Hence they can treat much larger systems

Accomplishments:

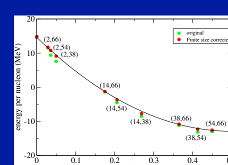
- Realistic NN intteractions using Chiral Interactions have been used to calculate the proprtie of selected closed shell nuclei
- The same AFDMC method has been used to calculate neutron matter, nuclear matter (isospin symmetric with N=Z, and matter with as a function of isospin.
- Realistic NNN interactions have been included in studies of neutron matter, work is proceeding for nuclei and nuclear matter

Impact

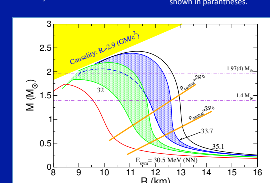
- Two nucleon interactions alone underbind Oxygen and all light nuclei, but overbind heavy nuclei and nuclear matter.
- Calculations of neutron matter place severe constraints on the Equation of State and the mass-radius relations of neutron stars, these will be tested in upcoming gravitational wave experiments.



Nuclear Matter with two different NN interactions. Calculations used up to 114 nucleons in periodic boundary conditions.



Energy versus proton fraction, from pure neutron matter (left) to N=Z nuclear mattter (right). Numbers of protons and neutrons are shown in parantheses.



Neutron Star Mass-Radius relations for NN interactions alone (red line) and for different three-nucleon interactions