LA-UR-93-3378

Title: MONTE CARLO STUDIES OF LIGHT NUCLEI:
STRUCTURE AND RESPONSE

Author(s): J. A. Carlson, T-5, Los Alamos National Laboratory

Submitted to: The Proceedings of the Few Body XIV Conference
Amsterdam, The Netherlands, August 23-28, 1993

MASTER

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

RECEIVED
OCT 07 1993
OSTI

Los Alamos
NATIONAL LABORATORY

Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the University of California for the U.S. Department of Energy under contract W-7405-ENG-36. By acceptance of this article, the publisher recognizes that the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. The Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy.

Form No. 836 R5
ST 2629 10/91

MONTE CARLO STUDIES OF LIGHT NUCLEI: STRUCTURE AND RESPONSE

J. Carlson
Theory Division
Los Alamos National Laboratory
Los Alamos, NM 87545

R. Schiavilla
Physics Department
Old Dominion University
Norfolk, VA 23529
and
Theory Group
Continuous Electron Beam Accelerator Facility
Newport News, VA 23606

Abstract

Monte Carlo methods based upon Euclidean path integrals can be used to study both structure and dynamics in few-body nuclei. Traditionally, these methods have been used in the limit of long imaginary time to extract information about low-lying states of light nuclei. Much intriguing dynamics, though, is present in the short time propagators. We briefly review some nuclear structure results, including bound-state results for $A=4$ and low-energy scattering for $A=5$. We stress recent developments related to inclusive processes, in particular calculations of the longitudinal and transverse response functions measured in electron scattering experiments. Calculations performed during the last year offer a much clearer picture of nuclear dynamics. In particular, they reproduce the observed quenching in the longitudinal to transverse response ratio, and the relative shift of strength to higher energies between the isoscalar and isovector responses probed in hadronic reactions.

Introduction

Monte Carlo methods are ideally suited to treat the nuclear few-body problem. Both variational[1] and Green's function Monte Carlo[2] (GFMC) methods are commonly used to study nuclear ground states and low-energy scattering. Here we focus on GFMC or Euclidean path-integral methods. Recently these techniques have been exploited to study a variety of problems in nuclear dynamics, and that will be the main emphasis here. First, though, we will describe the methods briefly and review some low-energy results.

Euclidean methods involve a rotation of the evolution operator to imaginary time: $\exp[iH\tau] \rightarrow \exp[-H\tau]$. Since the propagator $\exp[-\tau H]$ is in general unknown, the exponential is broken up into a product of short-time propagators: $\exp[-H\tau] = \prod \exp[-H\Delta\tau]$, where $\Delta\tau = \tau/N$. These short-time or high-temperature propagators are approximated, and Monte Carlo methods used to evaluate the relevant matrix elements. Euclidean formulations are popular in many fields of physics, including lattice QCD and many disciplines of condensed matter physics. Finite-temperature methods have recently been applied to studies of the nuclear shell model.[3]

For few-body problems we are predominantly concerned with ground-state expectation values and transitions, hence it is advantageous to include whatever approximate knowledge we have of the wave function. The ground-state expectation value of an operator O is simply the $\tau \rightarrow \infty$ limit of :

$$\langle O \rangle = \frac{\langle \Psi_T | \exp[-H\tau/2] O \exp[-H\tau/2] | \Psi_T \rangle}{\langle \Psi_T | \exp[-H\tau] | \Psi_T \rangle}. \quad (1)$$

The better the trial wave function Ψ_T , the faster the asymptotic limit is reached. At a formal level, the difference between these zero-temperature calculations and finite-temperature algorithms used in condensed matter and lattice QCD is in the boundary conditions. There are huge practical differences between the algorithms, of course, but in each case one is attempting to exploit the natural description of quantum problems in terms of path integrals. Monte Carlo is simply a tool which makes this possible.

Nuclear Interaction

We consider a simple non-relativistic formulation of the few-nucleon problem with a Hamiltonian of the form:

$$H = \sum_i T_i + \sum_{i < j} V_{ij} + \sum_{i < j < k} V_{ijk} \quad (2)$$

The NN interaction V_{ij} is fit to two-nucleon scattering data and deuteron properties. The dominant feature of the nuclear interaction is the long-range one-pion-exchange potential (OPEP):

$$V_\pi = [Y_\pi(r)\sigma_i \cdot \sigma_j + T_\pi(r)S_{ij}]\tau_i \cdot \tau_j, \quad (3)$$

where $Y_\pi \propto \exp[-\mu r/r]$, and $T_\pi \propto [1 + 3/(\mu r) + 3/(\mu r)^2]Y_\pi(r)$. The σ operators are standard Pauli spin matrices and S_{ij} is the tensor operator. In a simple mean-field approach to nuclear matter, OPEP would give no contribution. However, in realistic calculations of both nuclear matter and light nuclei, it has been found that OPEP contributes roughly two-thirds of the potential energy.[4] Hence, the strong correlations induced by the NN potential and, particularly, by OPEP are an essential feature of any microscopic description of the nucleus. For example, the binding energies of the $A=3$ and 4 nuclei are only 8.5 and 28.3 MeV, yet the kinetic energies are roughly 50 and 100 MeV, respectively. One primary motivation of few-body nuclear physics is the study of these correlations, both theoretically and experimentally.

All the calculations described here employ a simplified version of the Argonne[5] NN interaction, called the AV8 for the number of operators it contains. Low partial waves are constructed to match those in the V14 model, but higher-order terms in the relative momenta are not included. Momentum-dependent terms are difficult to handle in simple path-integral Monte Carlo schemes, they essentially correspond to different effective masses in each two-body channel. These terms have been constructed to be small in the V14 model, hence we treat the difference between AV14 and AV8 in perturbation theory. The perturbation is about 0.15 MeV in $A=3$ nuclei and 0.9 MeV in the alpha-particle.

In addition to the NN interaction, we include the Urbana model VIII [6] three-nucleon interaction (TNI) in our calculations. It contains an attractive long-range two-pion exchange term plus a repulsive dispersive term. It is adjusted to reproduce the ^3H binding energy; the strength parameters are plausible but not derived in any real sense from a microscopic theory. In nuclear matter calculations it nearly reproduces the experimental saturation density but gives too little binding. While it provides a significant fraction of the nuclear binding, the TNI expectation value is still a relatively small fraction ($\approx 10\%$) of the NN interaction one.

Interestingly, these 'reasonable' parametrizations of the TNI also provide good fits to the alpha-particle binding energy.[7] One should not consider this a 'proof' that the TNI is responsible for the missing binding energy in $A=3$ and 4 nuclei, though, since other effects, including both non-localities in the interaction and relativistic corrections, might have a similar density dependence. Each of these effects is expected to be significantly more important in the $A=4$ than in the $A=3$ nuclei, simply because of the fact that there are four triplets in the alpha-particle as compared to one in the $A=3$ systems. However, no reliable estimate of their contribution is as yet available.

Ground State Methods and Results

The first step in any path integral calculation is to construct an accurate short-time propagator. The free propagator G^0 is defined as:

$$G^0(R, R') = \langle R | \exp[-H\tau] | R' \rangle = N \exp[-(R - R')^2 m / 2\tau], \quad (1)$$

it provides a diffusion between R and R' . In the limit $\tau \rightarrow 0$, $G^0 = \delta(R - R')$. It is useful to construct the approximate interacting propagator from:

$$G(R, R') = G^0(R, R') \mathcal{S} \prod_{i < j} \frac{g_{ij}(r_{ij}, r'_{ij})}{g_{ij}^0(r_{ij}, r'_{ij})}. \quad (5)$$

Again, in the limit $\tau \rightarrow 0$, the ratio $g_{ij}/g_{ij}^0 \rightarrow \exp[-\Delta\tau(V(r_{ij}) + V(r'_{ij}))/2]$. More accurate expressions for the propagators are used in the actual calculations, but the basic idea is the same.[2] Three-nucleon interactions are included in an obvious way.

Once the short-time propagators are derived, ground-state expectation values are obtained by evolving the system to large τ . The convergence of the calculation with τ depends upon both the trial wave function and the excited-states spectrum of the Hamiltonian. The binding energy obtained with and without the Urbana TNI models are shown in Table 1. As we noted above, the TNI provides a significant fraction of the alpha particle binding, but a relatively small fraction of the total potential energy. The results obtained here include Coulomb, and are consistent within the error estimates with results obtained by Kamada et al. in the Faddeev-Yakubovsky approach.[8]

Table 1: Binding energies (MeV) for various interaction models

Interaction	$\langle H \rangle$	Error
AV8	-25.03	(0.10)
AV14	-24.20	(0.20)
AV14+TNI-VIII	-28.30	(0.20)

In addition to the binding energy, one is also interested in other properties such as form factors, momentum distributions, etc. When considering electromagnetic properties of the nucleus, it is necessary to include charge and current operators associated with the nuclear interaction, particularly those due to pion exchange. Their contribution can be quite significant even at relatively small values of the momentum transfer.

In the approach by Schiavilla and Riska [9, 10] the leading two-body charge and current operators are constructed directly from the interaction model. In addition to these, other current operators as well, such as those associated with intermediate Δ -production, are included. These latter terms are parametrized in a plausible way, but are not constrained directly by the interaction model.

Figure 1)

Alpha-particle charge form factor (from Ref. [7])

The alpha-particle charge form factor obtained in this approach is shown in figure 1; similar figures for the trinucleons charge and magnetic form factors are shown in Ref. [6], they are in quite good agreement with experiment up to roughly $q=3 \text{ fm}^{-1}$. As is apparent in the figure, the two-body charge contributions are absolutely crucial in obtaining this agreement.

Low-Energy Scattering

It is also possible to treat low-energy scattering with Euclidean methods by converting a scattering problem into a bound state one. By enforcing a specific boundary condition and solving for the ground-state energy, the phase shift at that energy can be obtained. Changing the boundary conditions allows one to study the behavior of the phase shift as a function of energy. The method is described in some detail in references [11, 12].

We have, for example, studied the two low-lying P-wave resonances in ^5He . In figure 2 we show their energy for a nodal radius R_N of 12.5 fm. The ^5He system is the smallest one where one can directly observe an $L \cdot S$ splitting in the low-lying states. In the figure, the energies of the $J = 3/2^-$ and $1/2^-$ are shown as a function of imaginary time τ relative to the alpha-particle ground-state energy.

Figure 2) Low-lying P-wave resonances in ${}^5\text{He}$

Neutron-alpha scattering phase shifts are well-known, of course, so that one can easily determine the experimental energy suitable to the boundary condition imposed in the simulation. These energies are shown as the two horizontal bars in the figure. Experimentally, $R_N = 12.5$ fm nearly corresponds to the position of the resonance in the $J = 3/2^-$ channel.

The qualitative agreement between theory and experiment is quite good. In particular, most of the observed $L \cdot S$ splitting is obtained in these calculations. It appears that the TNI gives a significant contribution to this splitting, although it is difficult to assign a precise contribution to individual terms in the Hamiltonian since the problem is very much non-perturbative. The $J = 3/2^-$ and $1/2^-$ relative wave functions are quite different here.

Some quantitative differences remain, however. It appears likely that the present Hamiltonian is unable to give the precise position of the two resonances, both states lie a few tenths of an MeV above the experimental value in our calculations. One obvious shortcoming is the simple TNI model employed, particularly the spin-isospin independent dispersive repulsion. There is little reason to believe that the TNI should be state-independent at short distances. At this detailed level, it will also be fruitful to attempt to improve the treatment of non-local interaction terms, and to study the convergence obtained with different trial wave functions.

Inclusive Scattering

The applications described above all depend upon the large- τ or low-energy properties of the propagators. As we have only recently begun to fully appreciate,[13] there is a wealth of information available in the intermediate and short-time propagators as well, information that is directly relevant to inclusive scattering experiments.

Inclusive scattering is traditionally studied in the framework of response functions. The dynamic response function $S(k, \omega)$ represents the response of a system to a weakly-coupled probe $\rho(k)$:

$$S(k, \omega) = \sum_f \langle 0 | \rho^\dagger(k) | f \rangle \langle f | \rho(k) | 0 \rangle \delta(\omega - \omega_f - \omega_0). \quad (6)$$

The Euclidean response is simply the Laplace transform of the standard real-time response:

$$S(k, \tau) = \int d\omega \exp[-(\omega - \omega_0)\tau] S(k, \omega) \quad (7)$$

$$= \langle 0 | \rho^\dagger(k) \exp[-(H - \omega_0)\tau] \rho(k) | 0 \rangle. \quad (8)$$

It is obvious that $S(k, \tau)$ can be calculated directly in a path integral simulation.

At $\tau = 0$ the Euclidean response is simply the sum rule, while the derivatives with respect to τ correspond to energy-weighted sum rules. For finite τ , the Euclidean response provides a measure of the energy distribution. As τ increases, the higher-energy components of the system are gradually suppressed and one is left with the low-energy response. In the $\tau \rightarrow \infty$ limit $S(k, \tau)$ is just the square of the relevant nuclear form factor.

Replacing the full interacting propagator with the gaussian free-particle propagator leads to Euclidean equivalents of the standard PWIA response functions obtained from momentum distributions or spectral functions. In these approximations the coupling of the struck nucleon to the rest of the system is ignored. Momentum distribution based calculations assume that the remaining nucleons are at a single energy, while spectral function based calculations take into account the interactions among the residual nucleons. Neither of these approximations is very accurate at momentum transfers of 300-400 MeV/c, however, as we shall see.

We have recently calculated the Euclidean response functions for a variety of simple single-nucleon couplings and also for 'realistic' couplings to longitudinally and transversely polarized virtual photons. The former are mainly of pedagogical interest, while the latter can be directly compared to electron scattering data.

The single-nucleon couplings are simple enough to allow us to provide a physical picture of the final-state interactions. In figure 3, we show the alpha-particle response at $k=350$ MeV/c for the following single-nucleon couplings:

$$\rho_1(k) = \sum_i \exp[i\mathbf{k} \cdot \mathbf{r}_i] \quad (9)$$

$$\rho_p(k) = \sum_i \exp[i\mathbf{k} \cdot \mathbf{r}_i] \frac{1 + \tau_z(i)}{2} \quad (10)$$

$$\rho_\tau(k) = \sum_i \exp[i\mathbf{k} \cdot \mathbf{r}_i] \tau_z(i) \quad (11)$$

$$\rho_{\sigma\tau L}(k) = \sum_i \exp[i\mathbf{k} \cdot \mathbf{r}_i] \tau_+(i) [\sigma_i \cdot \mathbf{k}] \quad (12)$$

$$\rho_{\sigma\tau T}(k) = \sum_i \exp[i\mathbf{k} \cdot \mathbf{r}_i] \tau_+(i) [\sigma_i \times \mathbf{k}], \quad (13)$$

For each operator $\rho_0(\mathbf{k})$ there is an associated response $S_0(\mathbf{k}, \omega)$, here denoted nucleon, proton, isovector, spin longitudinal, and spin transverse, respectively. For clarity the responses have been multiplied by $\exp[k^2/(2m)\tau]$ in order to remove the trivial kinematics associated with quasi-elastic scattering: the response of an isolated nucleon would simply be one on this scale.

Figure 3) Alpha-particle Euclidean response for simple probes at 350 MeV/c

It is instructive to compare the nucleon (S_1) and proton (S_p) responses. The former is sensitive purely to the average propagation of nucleons. By inserting complete sets of position eigenstates and integrating over the solid angle $d\Omega_k$, $S_1(k, \tau)$ can be calculated as an average over paths of $\sum_{ij} j_0(k|\mathbf{r}_i - \mathbf{r}_j|)$, where $\mathbf{r}_i$ and $\mathbf{r}_j$ are the initial and final positions of nucleons i and j . The equivalent expression for the proton response includes only sums over the initial and final proton positions.

The charge-exchange terms in the nuclear interaction play a crucial role in differentiating the proton and nucleon responses. Consider a time $\Delta\tau$ of roughly 0.01 MeV^{-1} , corresponding to excitation energies of 100 MeV. In this 'time', the free-particle propagator describes a diffusion on a scale of 1 fm. The relevant charge-exchange matrix element is approximately 40 MeV, implying a $\approx 40\%$ chance of a proton exchanging charge with a neutron during this time. Thus the charge propagates much faster than the nucleons themselves. This rapid propagation in imaginary time implies a shift of strength to higher excitation energies in the proton response, and a consequent quenching in the region of the quasi-elastic peak.

If viewed in a simple one-body picture, this process would have to be described as a 'swelling' of the nucleon charge distribution or as a decrease in the nucleon's effective mass. In fact it is a simple consequence of nuclear dynamics, and therefore the effect depends strongly upon the probe. It is also strongly momentum-dependent: at very high momentum transfers the relevant time scale is very small and the charge-exchange process cannot compete with free-particle propagation.

A comparison of the Euclidean proton response to longitudinal electron scattering is shown in figure 4. Here we present only the inelastic response, the elastic contribution has been subtracted both from theory and experiment. On the left, we have simply performed a Laplace transform of the experimental data. The points with error bars correspond to a 'truncated' response which is assumed to be identically zero beyond the highest measured energy. We have also attempted to extrapolate the measured response to include the effects of the high-energy tails. This extrapolation is given by the dashed lines in the figure and is, by construction, consistent with the Euclidean response at $\tau = 0$. By $\tau = 0.015 \text{ MeV}^{-1}$, however, the extrapolation has no effect and we can directly compare experiment and theory.

Figure 4) Proton response at 300 MeV/c; imaginary and real-time.

The PWIA and GPMC results are also shown. The latter are represented as a plus or minus one sigma error band. The PWIA response is very different from the observed one, but the full calculation is in good agreement with the data. It is necessary to include the effects of charge-exchange final-state interactions in order to achieve this agreement.

On the right, we have used a fitting procedure to extract the dynamic response from the Euclidean calculations. This procedure is described in reference [13], it essentially entails a fit to the difference between the PWIA and full calculations.

This charge-exchange mechanism naturally implies an even stronger shift and quenching in the purely isovector channel. For an isoscalar probe like the alpha-particle, the proton response is just the average of the nucleon and isovector responses. This shift is observed in our calculations, the pure isovector response in figure 3 can be obtained as a weighted average of the spin-longitudinal and spin-transverse isovector responses.

A strong shift is also observed with hadronic probes. Recent (p,n) measurements show a response shifted to energies much greater than $k^2/2m$. [14] The shift is a general

feature for all nuclei studied to date; it is also present for a variety of momentum transfers (figure 5). We note that the same shift is not apparent in (p,p') reactions, confirming the charge-exchange components of the NN interaction as the source of the shift.

Figure 5) Centroid of (p,n) and (p,p') quasi-elastic response. The solid line represents the free-particle energy of $k^2/2m$.

Given the predominantly isovector character of the one-body nuclear current, one would also expect to see a large quenching in the transverse response. Clearly this quenching is not observed in the experiments. In fact, the 'scaled' alpha-particle transverse response is roughly 20 % higher than the longitudinal one in the region of the peak. Using only the one-body current operators, the calculations are far below the experimental data. This is a simple consequence of the charge-exchange mechanism of the nuclear interaction.

In order to obtain a meaningful comparison with the data, the currents associated with this charge-exchange mechanism must also be included. We plot the data and the results of our calculations in figure 6. The data plotted here is truncated at the highest experimental value of the Bates[15] and Saclay [16] experiments, respectively. Since the Saclay experiment extends to higher ω , it will naturally lead to a larger Euclidean response near $\tau = 0$. The difference between Bates and Saclay at high τ is related to a fairly small relative energy shift in the two experiments.

Figure 6) Transverse response at 300 and 400 MeV/c, experiment vs. theory

We have used the current operators described in Ref. [9] for these calculations. The dominant corrections are expected to be those due to the pion currents, but our calculations include the remaining terms as well. In particular, they also contain a static description of the currents associated with delta production. This static model should be adequate at low energies, but obviously is not sufficient for high energies. In the transverse channel, this simplified theory can be directly compared to experiment for $\tau \geq 0.015 \text{ MeV}^{-1}$.

The calculated responses are found to be in good agreement with the experimental results. In order to achieve this agreement, it is absolutely essential to include realistic treatments of both final state interactions and current operators. Only in this way can one simultaneously understand the quenching in the longitudinal channel, the excess strength in the transverse channel, and the large shift observed with hadronic probes.

Conclusion

Path-Integral Monte Carlo techniques are a useful tool for studying both structure and dynamics in light nuclei. We have employed these techniques to make a convincing case for the consistency between experiment and a microscopic theory based upon realistic nuclear interactions and currents. Both ground-state expectation values and inclusive processes are well described in this framework.

We are currently exploring a variety of extensions to this work, including studies of larger nuclei, extraction of the dynamic response, calculations of polarization observables, and extensions to the higher-energy regime. There remains a large variety of intriguing few-body physics to be pursued with Monte Carlo methods.

References

- [1] J. Carlson, R. B. Wiringa, and V. R. Pandharipande, Nucl. Phys. **A410**, 59 (1983). J. Carlson and R. B. Wiringa, in *Computational Nuclear Physics Vol 1*, K. Langanke, J. A. Maruhn, and S. E. Koonin, eds., Springer-Verlag, Berlin, (1991).
- [2] J. Carlson, Phys. Rev. **C38**, 1879 (1988); Nucl. Phys. **A508**, 141c (1990).
- [3] C. W. Johnson, S. E. Koonin, G. H. Lang, and W. E. Ormand, Phys. Rev. Lett. **69** 3157 (1992).
- [4] S. C. Pieper and V. R. Pandharipande, Phys. Rev. **C 46** 1741 (1992).
- [5] R.B. Wiringa, R.A. Smith and T.L. Ainsworth, Phys. Rev. **C29**, 1207 (1984).
- [6] R.B. Wiringa, Phys. Rev. **C41**, 1585 (1991).
- [7] J. Carlson, Nucl. Phys. **A522**, 185c, (1991).
- [8] W. Glöckle and H. Kamada, Phys. Rev. Lett. **71**, 971 (1993).
- [9] R. Schiavilla, V.R. Pandharipande and D.O. Riska, Phys. Rev. **C40**, 2294 (1989); Phys. Rev. **C41**, 309 (1990).
- [10] J. Carlson, V.R. Pandharipande and R. Schiavilla, 'Modern Topics in Electron Scattering', B. Frois and I. Sick, eds., World Scientific, Singapore (1991), p. 177.
- [11] J. Carlson, V. R. Pandharipande, and R. B. Wiringa, Nuclear Physics **A424**, 47 (1984).
- [12] J. Carlson, K. E. Schmidt, and M. H. Kalos, Phys. Rev. **C36**, 27 (1987).
- [13] J. Carlson and R. Schiavilla, Phys. Rev. Lett **68**, 3682 (1992).
- [14] T. N. Taddeucci and J. B. McClelland, private communication.
- [15] K.F. von Reden et al., Phys. Rev. **C41**, 1084 (1990).
- [16] J.F. Danel et al., unpublished; J. Morgenstern, private communication.

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

END

DATE
FILMED

12 / 2 / 93