MONTE CARLO METHODS FOR NUCLEAR STRUCTURE

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1. Introduction

This talk is about some new and powerful methods for dealing with the nuclear shell model. These Monte Carlo methods, which have been developed at Caltech during the past five years, arise from a confluence of improvements in both algorithms and computer power. For selected observables, they allow calculations much larger and more realistic than any possible by other methods. The applications to date demonstrate the power and potential of the methods and the results in hand already offer a number of interesting physical insights, which I will describe to you. In addition, the path is now clear enough to project with some certainty further developments and accomplishments in these matters during the next few years.

My presentation is organized as follows. First, I will tell you what Shell Model Monte Carlo (SMMC) methods are capable of—what we can (and cannot) calculate. I would then like to give you some feeling for the general strategy of the calculations—how one deals with Hilbert spaces whose dimensions run to billions or more. My main focus will be on the application of these methods to problems of physical interest. In particular, I will discuss complete pf-shell calculations of both the ground state and thermal properties of Fe-peak nuclei. I will then turn to two topics in collective motion: the behavior of a hot, spinning rare-earth nucleus and of γ-soft nuclei near $A = 124$. I will also show you how these methods can be used to calculate two-neutrino double-beta decay rates. Finally, I will offer some thoughts on how this work will evolve over the next few years. I will emphasize the basic ideas and physics results throughout; the development and details of the method can be found in some of the early papers$^1$, as well as in a forth-coming review article$^2$.

2. What We Can Calculate

The SMMC methods I will describe are well suited to calculating thermal averages of observables. We cannot calculate the properties of any specific state, except for the ground state (which is obtained by going to very low temperature). Although this precludes detailed spectroscopy, it is not as limiting as it might seem. Inclusive reactions and astrophysical applications require the properties of nuclei at finite temperatures, and the exact ground state carries such interesting information as sum rules, pair correlations, etc.

Within these thermal ensembles we can calculate averages of few-body observables. Most of the interesting physics can be had from the one- and two-body density matrices, although the double beta-decay calculation described in Section 8 requires a four-body observable. The lack of explicit wavefunctions is

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1. See references in the text.
2. See references in the text.
not too much of a handicap, as the billions of amplitudes are of little interest in themselves. (After all, what experiment has ever measured a wavefunction!)

In addition to static observables, we can calculate information about the strength functions for one-body operators:

\[
S_A(\omega) = Z^{-1} \sum_{if} e^{-\beta E_i} \delta(\omega - E_f + E_i) |\langle f | A | i \rangle|^2
\]

(1)

where \(A\) is the operator of interest, \((i, f)\) are exact many-body eigenstates with energies \(E_{(i, f)}\), \(\beta\) is the inverse temperature, and \(Z\) the nuclear partition function; spectral functions (where \(A\) is an annihilation or creation operator) can also be calculated. The strength functions are obtained from the Laplace transform of the corresponding imaginary-time response functions. While the gross features of strength distributions are readily obtained, fine detail is quite difficult, but this is often quite commensurate with the experimental resolution.

SMMC results can be obtained with fully realistic shell model hamiltonians (for example, those derived from a \(G\)-matrix), although schematic interactions have been used as well. Most of the results I will show you include all configurations in one major shell, and multi-shell calculations are just beginning. Our confidence in the validity of the SMMC results (within the quoted uncertainties and the defined model) is based on careful comparisons with the results of more conventional methods, where the latter are feasible.

3. General Strategy

Let me now give you some feel for the general strategy by which we circumvent the combinatorial explosion of effort required in conventional shell model methods. As I mentioned, we consider thermal averages in the canonical (fixed-number) ensemble at an inverse temperature \(\beta\): \(\langle A \rangle = \text{Tr} \left( e^{-\beta H} A \right) / \text{Tr} e^{-\beta H} \).

The two-body interactions in the hamiltonian \(H\) cause all of the trouble; if \(H\) were pure one-body with \(N_s\) single-particle states, the trace over all many-body states could be readily evaluated by manipulations of \(N_s \times N_s\) matrices. The “trick” in SMMC is to transform the many-body problem into an infinite set of one-body problems, each in a different external field. The quantum mechanics of each of these is now quite tractable, but the price to be paid is the necessity to perform a weighted sum over all possible field configurations.

This latter task is handled by Monte Carlo methods, where only a statistical sample of the most important field configurations is considered. The calculations are done on massively parallel computers, where each computational node is tasked to produce and analyze a few field configurations, and the final result is obtained by averaging over all nodes. The statistical uncertainty decreases as the square-root of the number of samples; typically several thousand yield the required precision. In contrast to conventional diagonalization methods, the numerical effort in SMMC is independent of the number of valence nucleons involved and scales only as \(N_s^3\).
4. Ground States in the Fe Region

The first applications I will discuss are the properties of 28 nuclei (even-even Ti, Cr, Fe, Ni, and Zn isotopes, together with odd-odd \( N = Z \) nuclides) in the Fe region. The single-particle orbitals used were the 1p0f-shell (\( N_s = 20 \)) and the Hamiltonian was the Kuo-Brown interaction (KB3) with a tiny monopole adjustment. The calculations were done at \( T = 0.5 \text{ MeV} \), which experience has shown to be sufficiently large so that observables correspond essentially to ground-state properties.

Fig. 1: Upper panel: experimental and calculated mass defects. Lower panel: Errors in the SMMC mass defects. The horizontal lines show the average (solid) and rms (dashed) errors; a typical SMMC uncertainty is indicated.

Fig. 2: Calculated and experimental \( E2 \) strengths. Open circles show the experimental \( 0^+_1 \rightarrow 2^+_1 \) values, while solid squares show the experimental total values.

As shown in Fig. 1, the Coulomb-corrected mass defects are in excellent agreement with experiment, the average error being +0.45 MeV (this is consistent with the average internal excitation energy expected). Figure 2 shows the calculated total \( B(E2) \) strengths, using effective charges \( (e_p, e_n) = (1.35, 0.35) \) that are consistent with conventional shell-model experience. Comparisons with experimental values for only the lowest \( 2^+ \) state are good, and the agreement with the total strengths, where available from electron scattering, is excellent.

The individual \( j \)-shell occupations in the Fe isotopes are shown in Fig. 3.

The successive neutrons generally occupy the higher orbitals, although the influence of the \( f_{7/2} \) shell closure in \(^{54}\text{Fe} \) is evident, as is the effect of the neutron-proton interaction on the proton occupations. To get some sense of the coherence in the ground states, one can consider the proton BCS pairing gap, \( \langle \Delta_p^+ \Delta_p \rangle \), where \( \Delta_p^+ = \sum P_{jm}^+ P_{jm}^\dagger \), the sum being over all orbitals with \( m > 0 \); the neutron gap is defined analogously. Figure 4 shows the proton and neutron gaps for the Fe, Ni, and Zn isotopes relative to those calculated for a Fermi gas with the same occupation numbers. The proton pairing increases as neutrons are added, while the neutron pairing clearly shows the \( f_{7/2} \) shell closure. A broader (and less model-dependent) view of pair correlations can be had by defining the operators \( A_j^\dagger \equiv [a_j^\dagger \times a_j^\dagger]_{JM} \) for each pair of orbitals, and then diagonalizing the matrix \( \langle A_j^\dagger A_{JM} \rangle \) for each \( J \). For \( J = 0 \), the largest eigenvalue far exceeds the others, and defines the “optimal” pair content and wavefunction. As discussed in Section 7 below, channels with \( J > 0 \) can also show meaningful coherence.

Fig. 3: Calculated occupation numbers in the ground states of the Fe isotopes. Error bars are generally too small to be shown.

Fig. 4: Proton and neutron gaps (relative to the Fermi gas values) for the Fe, Ni, and Zn isotopes.
Fig. 5: Experimental and calculated GT\(^+\) strengths. Discrepancies for \(^{48}\)Ti and \(^{64}\)Ni are likely due to deficiencies in the model space used.

Particularly significant are the SMMC results for the total Gamow-Teller (GT) strengths, \(B(\text{GT}) = \langle G_\mp G_\pm \rangle\), with \(G_\pm = \sum \sigma T_\pm\) the usual GT operator. \(B(\text{GT})\) as measured in forward \((n,p)\) reactions is typically only some 30\% of the independent particle estimate. The Monte Carlo results shown in Fig. 5 resolve this discrepancy: the complete shell-model calculations systematically reproduce the experimental values, provided the former are normalized by \(0.64 = (1/1.25)^2\). This is consistent with in-medium quenching of the axial charge to \(g_A = 1\), as \(\beta\)-decay matrix elements are used to normalize the experimental \((n,p)\) results. A similar situation holds in the \(sd\)-shell. These data also show that \(B(\text{GT})\) is proportional to the numbers of valence protons and valence neutron holes, so that the four \(pf\)-orbitals apparently behave as one large entity.\(^4\)

The extent to which the agreement between the data and the SMMC results survives (or can be improved) with other hamiltonians or larger model spaces will be explored in the near future.

5. Thermal Properties of Fe-Peak Nuclei

To investigate thermal properties, we have considered nuclei near Fe at finite temperature. The calculations\(^5\) include the complete set of \(1p0f\) states interacting through the realistic Brown-Richter or Kuo-Brown Hamiltonians.

Fig. 6: Temperature dependence of various observables in \(^{54}\)Fe. Shown in the left-hand column are the internal energy, \(U\), the heat capacity \(C\), and the level density parameter \(a\). In the right-hand column are the neutron and proton pairing fields (values calculated in an uncorrelated Fermi gas are shown by the solid curves) and the moment of inertia, \(I = \beta\langle J^2 \rangle / 3\).

The calculated temperature dependence of various observables in \(^{54}\)Fe is shown in Fig. 6. The internal energy \(U\) increases steadily with increasing temperature. It shows an inflection point around \(T \approx 1.1\) MeV, leading to a peak in the heat capacity, \(C \equiv dU/dT\). The decrease in \(C\) for \(T \gtrsim 1.4\) MeV is due to the finite model space (Schottky effect); the limitation to only the \(pf\)-shell renders the calculations quantitatively unreliable for temperatures above this value (internal energies \(U \gtrsim 15\) MeV). The same behavior is apparent in the level density parameter, \(a \equiv C/2T\). The empirical value for \(a\) is \(A/(8\ \text{MeV}) = 6.8\ \text{MeV}^{-1}\), which is in good agreement with the results for \(T \approx 1.1\)–1.5 MeV.

Fig. 7: Temperature dependence in \(^{54}\)Fe of the total magnetic dipole strength \(B(M1)\) (calculated using free-nucleon \(g\)-factors), Gamow-Teller strength, and isoscalar and isovector quadrupole strengths.
Also shown in Fig. 6 are the proton-proton and neutron-neutron BCS pairing fields, $\langle \Delta^\dagger \Delta \rangle$. At low temperatures, the pairing fields are significantly larger than those calculated for a non-interacting Fermi gas. With increasing temperature, the pairing fields decrease, approaching the Fermi gas values for $T \approx 1.5$ MeV and following it closely for even higher temperatures. Associated with the breaking of pairs is a dramatic increase in the moment of inertia, $I$, for $T = 1.0$–1.5 MeV. At temperatures above 1.5 MeV, $I$ is in agreement with the rigid rotor value, $10.7h^2/\text{MeV}$; at even higher temperatures it decreases linearly due to the finite model space.

Some other static observables are shown in Fig. 7. The magnetic dipole strength, $B(M1)$, unquenches rapidly with heating near the transition temperature, but remains significantly lower than the single-particle estimate ($41 \mu^2_N$) for $T = 1.3$–2 MeV, suggesting a persistent quenching at temperatures above the like-nucleon depairing. This finding is supported by the near-constancy of $B(GT_+)$ for temperatures up to 2 MeV, as is often assumed in astrophysical calculations. Detailed study of pairing observables shows that these behaviors are driven largely by the rapid vanishing of the like-nucleon $J = 0$ pairing near $T = 1.1$ MeV and a peaking of the unlike $J = 1$ pairing near $T = 2.25$ MeV.

Fig. 8: $GT_+$ response functions (left) and corresponding strength distributions (right) at temperatures of roughly 1 MeV. Data from $(n, p)$ reactions are shown as histograms and the vertical lines indicate the centroids used in current astrophysical calculations.

The $GT_+$ strength distributions $S(E)$ can be obtained as the inverse Laplace transform of the response function $R(\tau) = \langle G_-(\tau)G_+(0) \rangle$, where the GT operators are in the imaginary-time Heisenberg picture. Figure 8 shows these quantities for $^{51}$V, $^{59}$Co, and $^{55}$Co. Reasonable agreement is found with the $(n, p)$ data for the first two nuclei (the calculations have not yet been folded with the experimental energy resolution). That the centroid in the third case is significantly higher than that predicted by Fuller et al. indicates that an important presupernova electron capture rate is likely significantly slower than the currently accepted value.

In a related study, SMMC calculations have been applied to test a suggestion that the nuclear symmetry energy increases with temperature due to a decrease in the nucleon effective mass. If true, this would decrease supernova electron-capture rates. To test this hypothesis, we performed SMMC calculations of the differences in internal energies for several pairs of even-even isobars at finite temperatures. The calculations generally do not support a temperature-dependent increase in the symmetry energy.

Finite temperature SMMC calculations for other nuclei in this mass range show behavior similar to that of $^{54}$Fe; the qualitative features are also similar when other realistic interactions are used. Results at temperatures above 1.5 MeV will become reliable only when two or more major shells are included in the calculations. The extension of these studies to other interactions, heavier nuclei, and other observables
will allow a more thorough understanding of nuclear properties at high excitation energies.

6. $^{170}$Dy at Finite Temperature and Spin

The results of a calculation for $^{170}$Dy demonstrate what SMMC methods can bring to the description of heavier nuclei. The protons occupied the $Z = 50–82$ shell while the neutrons were in the $N = 82–126$ shell ($N_s$ was thus 32 and 44, respectively). The nucleus $^{170}$Dy is of no special interest physically, but as it is mid-shell in this model space (16 valence protons and 22 valence neutrons), it is the most challenging (there are some $10^{21}$ $m$-scheme determinants). The hamiltonian was of the conventional pairing plus quadrupole form. Both grand-canonical (fixed chemical potential) and canonical ensembles were used (and found to be quite similar) and finite rotations were investigated by adding a cranking term $-\omega J_z$ to the hamiltonian.

Fig. 9: Grand-canonical observables for $^{170}$Dy at various cranking frequencies and temperatures. Shown are the average sign $\langle \Phi \rangle$ (a smaller value indicates a numerically more difficult calculation), the square of the isoscalar quadrupole moment $\langle Q^2 \rangle$, the energy $\langle H \rangle$, the square of the angular momentum $\langle J^2 \rangle$, the dynamical moment of inertia $I_2 = d\langle J_z \rangle/d\omega$, and the expectation value of the pairing terms in the hamiltonian, $-g \langle \hat{P}^\dagger \hat{P} \rangle$. Error bars not shown are approximately the size of the symbols, and lines are drawn to guide the eye.

Fig. 10: Contours of the free energy in the polar-coordinate $\beta - \gamma$ plane for $^{170}$Dy. Contours are shown at 0.3 MeV intervals, with lighter shades indicating the more probable nuclear shapes.

The systematics of the cranked system are shown in Fig. 9. At high temperatures, the nucleus is unpaired and the moment of inertia decreases as the system is cranked. However, for lower temperatures when the nucleons are paired, the moment of inertia initially increases with $\omega$, but then decreases at larger cranking frequencies as pairs break; the pairing gap also decreases as a function of $\omega$. It is well known that the moment of inertia is suppressed by pairing and that initially $I_2$ should increase with increasing $\omega$. Once the pairs have been broken, the moment of inertia decreases. These features are evident in the figure.
In addition to simple observables, the nuclear shapes were calculated from the mass quadupole tensor of each Monte Carlo sample; the free energy can be extracted from the distribution of these shapes. Figure 10 shows the temperature evolution of the free-energy surface. At high temperatures, the system is nearly spherical, whereas at lower temperatures, especially at $T = 0.3$ MeV, there is a prolate minimum on the $\gamma = 0$ axis.

Further systematic investigations of this sort are underway and expansion of the single-particle basis to several major shells does not seem impossible.
7. Gamma-Soft Nuclei

The ground states of nuclei with $A \sim 124$ are expected to have large shape fluctuations. In geometrical terms, the potential energy surface has a minimum at finite $\beta$, independent of $\gamma$; in the Interacting Boson Model, there is at $O(6)$ dynamical symmetry. Recent SMMC work$^9$ has provided the first microscopic many-body description of this phenomenon.

Valence protons and neutrons were assumed to occupy the 50-82 shell (i.e., $N_s = 32$). Single particle energies were taken from a spherical Woods-Saxon potential and the two-body interaction involved both monopole and quadrupole pairing, as well as the usual $QQ$ term. The parameters of the Hamiltonian were adjusted to reproduce the experimental pairing energies and excitation energies and $B(E2)$ values of the $2^+_1$ states. Rotations were investigated by cranking with $-\omega J_z$.

Fig. 11: Cranking response of $^{124}$Xe and $^{128}$Te at temperatures $T = 0.5$ and 0.33 MeV. Shown are the dynamical moment of inertia, $I$, the mass quadrupole strength, the proton pairing strength, and $\langle J_z \rangle$.

Fig. 12: Similar to Fig. 10 for $^{124}$Xe and $^{128}$Te at temperatures $T = 1.0$, 0.5, and 0.33 MeV.

The rotational responses of $^{124}$Xe (4 valence protons and 20 valence neutrons) and $^{128}$Te (2 protons and 26 neutrons) at two different temperatures are shown in Fig. 11. The $\omega = 0$ inertia for both nuclei is significantly lower than the rigid body value ($\sim 43h^2$/MeV) and increases with increasing rotation as the pairing decreases. Peaks in $I_2$ are associated with the onset of deformation as measured by $\langle Q^2 \rangle$. This suggests a band crossing associated with pair breaking and alignment, as is known to occur in $^{124}$Xe near spin $10\hbar$. The alignment is clearly seen in the behavior of $\langle J_z \rangle$ at the lower temperature, which shows a rapid increase after an initial moderate growth. Both deformation and pairing decrease with increasing temperature.

Calculated free energies for $^{124}$Xe and $^{128}$Te are shown in Fig. 12. Both nuclei are essentially spherical at high temperature, but become $\gamma$-soft at low temperature, with minima at $\beta \sim 0.15$ and 0.06, respectively. $^{128}$Te appears to be prolate, while $^{124}$Xe seems to be nearly $\gamma$-unstable.

A crude point of contact with the IBM can be had by calculating the numbers of correlated $J = 0$ and $J = 2$ pairs (i.e., excesses beyond the mean-field values) at low temperature and comparing them with the expected numbers of $S$ and $D$ bosons. For $^{124}$Xe, the SMMC (IBM) results for protons are 0.85 (1.22) $S$-pairs and 0.76 (0.78) $D$-pairs, where the IBM values correspond to the exact $O(6)$ limit. For neutron holes in the same nucleus, the corresponding values are 1.76 (3.67) $S$-pairs and 2.14 (2.33) $D$-pairs. For protons, the $D/S$ ratio of 0.89 is not far from the $O(6)$ value of 0.64, while for neutron holes, the $D/S$ of 1.21 is intermediate between $O(6)$ and $SU(3)$ (where it is 1.64), as is consistent with neutrons filling the middle of the shell. Although the total numbers of $S$ and $D$ pairs in the SMMC calculations
8. Double Beta Decay

The second-order weak process \((Z, A) \rightarrow (Z + 2, A) + 2e^- + 2\bar{\nu}_e\) is an important “background” to searches for the lepton-number violating neutrinoless mode, \((Z, A) \rightarrow (Z + 2, A) + 2e^-\). The calculation of the nuclear matrix elements for these two processes is a challenging problem in nuclear structure, and has been done in a full \(pf\) model space with conventional methods only for the lightest of several candidates, \(^{48}\text{Ca}\).

The required matrix element for \(2\nu\) decay is

\[
M_{2\nu} = \sum_n \frac{\langle f|G_-|n\rangle \langle n|G_-|i\rangle}{\Omega - E_n} \tag{2}
\]

Here, \((i, f)\) are the \(0^+\) ground states of the parent and daughter nuclei, \(\Omega\) is the average of their energies, and the sum is over all \(1^+\) states, \(n\), of the intermediate nucleus with energies \(E_n\). The difficulties in a direct diagonalization approach involve knowing the exact wavefunctions of the states involved, performing the sum over all intermediate states, and the large cancellations that occur among the various terms in the sum.

To calculate \(M_{2\nu}\) in very large model spaces with SMMC methods, one considers the observable\(^{10}\)

\[
F(\tau_1) = \frac{\text{Tr}[e^{-(\beta - \tau - \tau_1)H}G_+G_+e^{-\tau H}G_-e^{-H\tau_1}G_-]}{\text{Tr}e^{-\beta H}}. \tag{3}
\]

If both \(\beta\) and \(\tau\) are sufficiently large to filter out the parent and daughter ground states, setting \(\tau_1 = 0\) leads to the usual closure matrix element, \(M_c = \langle f|G_-G_-|i\rangle\), while integrating over \(\tau_1\) generates the required intermediate-state energy denominator and hence leads to the exact \(M_{2\nu}\).

A first calculation to validate the SMMC method against direct diagonalization results has been performed for \(^{48}\text{Ca}\). There is good agreement between the SMMC and conventional results for the closure and exact matrix elements; cancellations make the matrix element for \(^{48}\text{Ca}\) anomalously small, and hence the calculation particularly demanding. A similar calculation for \(^{76}\text{Ge}\) in the \(1p0f_{5/2}0g_{9/2}\) model space is in progress. Of particular interest will be the sensitivity to the effective interaction, the overlap of GT\(_+\) and GT\(_-\) strengths in the intermediate nucleus, and the validity of both the closure approximation and the more sophisticated quasi-particle RPA. Candidates for follow-on calculations include \(^{82}\text{Se}\), \(^{96}\text{Zr}\), \(^{100}\text{Mo}\), \(^{128,130}\text{Te}\), and \(^{136}\text{Xe}\).

9. Summary and Outlook
I have presented a sampling of results from Shell Model Monte Carlo calculations. These demonstrate both the power and limitations of the methods and the physical insights they offer. SMMC calculations, while not a panacea, clearly have certain advantages over conventional shell model approaches, particularly for properties of ground states or thermal ensembles. Of the results I have discussed, the most significant bear on the quenching of GT strength, on the pairing structure, and on nuclear shapes.

With respect to the technical aspects of these calculations I note the following:

1) SMMC methods are computationally intensive. However, computing power is becoming cheaper and more widely available at an astonishing rate. It is a great advantage that these calculations can efficiently exploit loosely connected “farms” of work-station-class machines.

2) We already have strong circumstantial evidence that center-of-mass (CM) motion is not a significant concern for many of the operators of interest (the $E1$ operator being an outstanding exception). This is not too surprising at finite temperature, since the CM is only three degrees of freedom (far fewer than the internal dynamics). Indeed, multi-shell calculations have been initiated.

3) We lack the ability to treat odd-$A$ or odd-odd $N \neq Z$ systems at low temperatures because of “sign” problems in the Monte Carlo sampling. Similar problems prevent spin projection, which would enable yrast spectroscopy. Work to circumvent these problems is clearly needed.

4) Otsuka and collaborators\textsuperscript{11} have recently proposed a hybrid scheme whereby SMMC methods are used to select a many-body basis, which is then employed in a conventional diagonalization. The sign problems alluded to above are absent, and detailed spectroscopy is possible. Test applications to boson problems have shown some promise, although the utility for realistic fermion systems remains to be demonstrated.

Additional physics results that should emerge in the next year or two include: more realistic electron capture rates in pre-supernova conditions, the two-neutrino double-beta decay matrix elements for $^{76}$Ge, and $^{128,130}$Te, systematic studies of rare earth nuclei at finite temperature and spin, studies to improve the effective interactions used, tests of such models as the IBM and RPA, and predictions of nuclear properties far from $\beta$-stability. There are undoubtedly interesting applications beyond these, and suggestions are welcome.

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