Shell model Monte Carlo calculations
for $^{170}$Dy

D. J. Dean, S. E. Koonin, G. H. Lang, P. B. Radha, and W. E. Ormand

W. K. Kellogg Radiation Laboratory, California Institute of Technology,
Pasadena, CA 91125 USA

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Abstract

We present the first auxiliary field Monte Carlo calculations for a rare earth nucleus, $^{170}$Dy. A pairing plus quadrupole Hamiltonian is used to demonstrate the physical properties that can be studied in this region. We calculate various static observables for both uncranked and cranked systems and show how the shape distribution evolves with temperature. We also introduce a discretization of the path integral that allows a more efficient Monte Carlo sampling.
I. INTRODUCTION

Although mean-field models of rare-earth nuclei can describe the gross interplay between collective and single-particle degrees of freedom [1], it is of obvious interest to pursue a fully microscopic description to the greatest extent possible, particularly as the angular momentum and/or temperature is increased. As we have previously developed and demonstrated Monte Carlo methods for treating very large basis shell model calculations [2,3], it is natural to attempt to extend them to the rare-earth region. Toward this end, we present here the first auxiliary field Monte Carlo calculations of observables in a rare-earth nucleus. For demonstration purposes, we have chosen the pairing plus quadrupole Hamiltonian and consider the mid-shell nucleus $^{170}$Dy.

As we move up to the rare earth region from the $sd$- and $fp$-shell spaces, new physical and computational problems must be solved. The neutrons and protons occupy different major shells, and so isospin symmetry is lost. Further, the numbers of single-particle orbitals and valence particles are larger. Most importantly, the long autocorrelations times encountered in Metropolis sampling [3,4] of continuous auxiliary fields have to be avoided by a novel discretization of the fields based on gaussian quadrature. The small level spacing of these larger nuclei also requires calculations at lower temperatures.

Our presentation is organized as follows. In Section II we review the auxiliary field Monte Carlo method, discuss our choice of the Hamiltonian, and introduce a discretization of the path integral to facilitate the Monte Carlo sampling. We present results of static observables and deformation distributions for $^{170}$Dy at various temperatures and cranking frequencies in Section III, and draw several conclusions about future directions.

II. FORMALISM

Details of the auxiliary field Monte Carlo approach to the shell model have been presented elsewhere [2,3], so that we only outline the method here. Given some many-body
Hamiltonian $H$, we desire a tractable expression for the imaginary time evolution operator,

$$U = \exp (-\beta H) ,$$  \hspace{1cm} (2.1)

where $\beta$ has units of inverse energy (MeV$^{-1}$, where $\hbar = 1$) and $\beta^{-1}$ can be interpreted as
the temperature of the system. The operator $H$ is a generalized many-body Hamiltonian,
and may contain terms such as $-\mu N$ in the grand-canonical ensemble, or $-\omega J_z$ in cranked
systems. (In these cases, $\mu$ is the chemical potential and $\omega$ is the cranking frequency.) The
partition function is

$$Z = \text{Tr} \exp (-\beta H) ,$$  \hspace{1cm} (2.2)

from which we can construct the thermal expectation value of an operator $O$ as

$$\langle O \rangle = \frac{1}{Z} \text{Tr} \left[ O \exp (-\beta H) \right] .$$  \hspace{1cm} (2.3)

Here, Tr is the trace over many-body states of fixed (canonical) or all (grand-canonical)
particle number.

We restrict ourselves to generalized Hamiltonians that contain at most two-body terms.
The Hamiltonian can then be written as a quadratic form in some set of convenient operators
$\{O_{\alpha}\}$,

$$H = \sum_{\alpha} \epsilon_{\alpha} O_{\alpha} + \frac{1}{2} \sum_{\alpha} V_{\alpha} O_{\alpha}^2 ,$$  \hspace{1cm} (2.4)

where we have written the quadratic term in diagonal form. These operators are typically
either one-particle (density) or one-quasiparticle (pairing), and the strength of the two-body
interaction is characterized by the real numbers $V_{\alpha}$ related to the two-body matrix elements.

For $H$ in the quadratic form (2.4), we can write the evolution operator as a path integral.
The exponential is first split into $N_t$ ‘time’ slices, $\beta = N_t \Delta \beta$, so that

$$U = \left[ \exp (-\Delta \beta H) \right]^{N_t} .$$  \hspace{1cm} (2.5)

A Hubbard-Stratonovich (HS) transformation is then performed on the two-body term
in each time slice $n = 1, \ldots, N_t$ yielding for the evolution operator
\begin{equation}
U = \left[ \exp \left( -\Delta \beta H \right) \right]^{N_t} \simeq \int \mathcal{D}[\sigma] G(\sigma) U_\sigma ,
\end{equation}

where the integration measure is
\begin{equation}
\mathcal{D}[\sigma] = \prod_{n=1}^{N_t} \prod_{\alpha} d\sigma_{\alpha n} \left( \frac{\Delta \beta | V_\alpha |}{2\pi} \right)^{1/2} ,
\end{equation}

the Gaussian factor is
\begin{equation}
G(\sigma) = \exp \left( -\sum_{\alpha n} \frac{1}{2} \Delta \beta | V_\alpha | \sigma_{\alpha n}^2 \right) ,
\end{equation}

the one-body evolution operator is
\begin{equation}
U_\sigma \equiv U_{N_t} U_{N_{t-1}} \ldots U_1 ,
\end{equation}

with \( U_n \equiv \exp \left[ -\Delta \beta h_\sigma (\tau_n) \right] \), and the one-body Hamiltonian is
\begin{equation}
h_\sigma (\tau_n) = \sum_{\alpha} (\varepsilon_\alpha + s_\alpha V_\alpha \sigma_{\alpha n}) O_\alpha ,
\end{equation}

where the phase factor \( s_\alpha \) is \( \pm 1 \) if \( V_\alpha < 0 \), and is \( \pm i \) if \( V_\alpha > 0 \). Each real variable \( \sigma_{\alpha n} \) is the auxiliary field associated with \( O_\alpha \) at the time slice \( n \).

Expectation values of observables are calculated through
\begin{equation}
\langle O \rangle = \frac{\int \mathcal{D}[\sigma] G(\sigma) \zeta(\sigma) \langle O \rangle_\sigma}{\int \mathcal{D}[\sigma] G(\sigma) \zeta(\sigma)} ,
\end{equation}

where
\begin{equation}
\zeta(\sigma) = \text{Tr} U_\sigma
\end{equation}
is the partition function for each field configuration and
\begin{equation}
\langle O \rangle_\sigma = \frac{\text{Tr} [OU_\sigma]}{\zeta(\sigma)} .
\end{equation}

To perform the integration via Monte Carlo methods, we introduce the non-negative integration weight \( W(\sigma) = G(\sigma) | \zeta(\sigma) | \), and the “sign” \( \Phi(\sigma) = \zeta(\sigma)/ | \zeta(\sigma) | \), so that the expression (2.11) for an observable becomes
\[
\langle \mathcal{O} \rangle = \frac{\int D[\sigma] W(\sigma) \Phi(\sigma) \langle \mathcal{O} \rangle_{\sigma}}{\int D[\sigma] W(\sigma) \Phi(\sigma)}.
\]

(2.14)

The integral (2.14) can be evaluated by Monte Carlo methods using samples generated by the algorithm of Metropolis et al. [4], as described in Ref. [3]. However, in view of the large number of auxiliary fields involved (some \(10^5\)), the successive field configurations are highly correlated for a reasonable acceptance fraction (\(\sim 0.5\)), the autocorrelation length being over 200 sweeps. To generate uncorrelated samples more efficiently, we have approximated the continuous integral over each \(\sigma_{\alpha n}\) by a discrete sum derived from a Gaussian quadrature. In particular, the relation

\[
e^{\Delta \beta V \mathcal{O}^2/2} \approx \int_{-\infty}^{\infty} d\sigma f(\sigma) e^{\Delta \beta V \sigma \mathcal{O}}
\]

(2.15)
is satisfied through terms in \((\Delta \beta)^2\) if \(f(\sigma) = \frac{1}{4} \left[ \delta(\sigma - \sigma_0) + \delta(\sigma + \sigma_0) + 4\delta(\sigma) \right]\), where \(\sigma_0 = (3/V \Delta \beta)^{1/2}\). (Note that commutator terms render the HS transformation accurate only through order \(\Delta \beta\) anyway.)

In this way, each \(\sigma_{\alpha n}\) becomes a 3-state variable and the path integral becomes a (very large) path sum, which can be sampled using the algorithm of Metropolis et al. We have found that this discretization reduces the correlation length to only five sweeps, and thus increases our efficiency by a factor of 40 relative to the continuous case, with no loss of accuracy.

To describe rare-earth nuclei, we choose the \(Z = 50–82\) shell for protons \((2s1d0g_7/20h_{11/2})\) and the \(N = 82–126\) shell for neutrons \((2p1f0g_{9/2}0i_{13/2})\). The Hamiltonian we have chosen is of the pairing plus quadrupole form given by

\[
H = \sum_{\alpha} \varepsilon_{\alpha} a_{\alpha}^\dagger a_{\alpha} - g_p P_p^\dagger P_p - g_n P_n^\dagger P_n - \frac{\chi}{2} Q_p \cdot Q_n,
\]

(2.16)

where \(\varepsilon_{\alpha}\) are the single particle energies, \(a_{\alpha}^\dagger\) and \(a_{\alpha}\) are the anti-commuting creation and annihilation operators associated with the single particle state \(\alpha\), \(P_p^{\dagger}\), \(P_p\) are the monopole pair creation and annihilation operators for protons and neutrons, and \(Q_p\) is the quadrupole-moment operator. The single particle states \(\alpha\) are defined by the complete
set of quantum numbers $nljmt_z$, denoting the principal, orbital angular momentum, total single-particle angular momentum, $z$-projection of $j$, and the third component of the isospin quantum numbers, respectively. Single-particle operators are thus represented by matrices of dimension 32 and 44, for protons and neutrons, respectively. The pairing strengths $g_{p(n)}$, the quadrupole interaction strength $\chi$, and the single particle energies used in our calculations are given in Table I (taken from Ref. [6]).

III. THE CALCULATION AND RESULTS

To demonstrate the power of our methods, we study the mid-shell nucleus $^{170}$Dy (16 valence protons and 22 valence neutrons), which requires some $10^{21}$ $m$-scheme determinants. We have used $\Delta \beta = 0.0625$ and $N_t = 8$ to 64 time slices.

In addition to grand-canonical calculations, we performed canonical analyses of the fields generated through grand-canonical sampling. In particular, canonical observables (subscript “$c$”) are given in terms of the grand-canonical sampling (subscript “$g$”) as

$$\langle O \rangle_c = \frac{\int \mathcal{D}[\sigma] W_g(\sigma) \Phi_c(\sigma) [\zeta_c(\sigma)/\zeta_g(\sigma)] \langle O \rangle_{c\sigma}}{\int \mathcal{D}[\sigma] W_g(\sigma) \Phi_c(\sigma) [\zeta_c(\sigma)/\zeta_g(\sigma)].} \quad (3.1)$$

The fluctuations in $[\zeta_c(\sigma)/\zeta_g(\sigma)]$ determine how precise this evaluation can be. We find that the fluctuations are less than 10% (as the number distribution in the grand-canonical ensemble is small), so that canonical observables can be calculated with good precision.

In Fig. (1) we show the static observables for the uncranked system in both the grand-canonical and canonical formalisms. We calculated observables canonically, using grand canonical fields, up to $\beta = 2.0$ in order to demonstrate that for these nuclear systems, either method may be used in this kind of calculation. Note that as the temperature decreases, the nucleus becomes more deformed. Relaxation of the expectation values of $H$ and $J^2$ is also clearly seen. The sign in these cases is identically one for all temperatures.

Cranking calculations in which $H \rightarrow H - \omega J_z$ have also been performed. The systematics are shown in Fig. (2) where we display $\langle \Phi \rangle, \langle H \rangle, \langle Q^2 \rangle, \langle J^2 \rangle, -g\langle P^+ P \rangle$, and the moment of
inertia, $\langle I_2 \rangle$. Note that the sign degrades quite rapidly with increasing $\omega$, making cranking calculations at lower temperatures difficult. Moments of inertia were calculated from $I_2 = d\langle J_z \rangle/d\omega = \beta[(\langle J_z^2 \rangle - \langle J_z \rangle^2)]$. 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 as we begin to crank, but then decreases at larger cranking frequencies as pairs break; Figure 2 shows that the pairing gap also decreases as a function of $\omega$. It is well known that the moment of inertia depends on the pairing gap [7], 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 static observables, we have calculated the nuclear shape distributions. These distributions give a clear description of various shape and phase transition phenomena [8]. To obtain a detailed picture of the deformation, we use the components of the quadrupole operator $Q_\mu = r^2Y_{2\mu}^*$. Rotational invariance of the Hamiltonian implies that the expectation value of each component of $Q_\mu$ vanishes on average; however, each Monte Carlo sample will have finite $Q_\mu$ values, from which we construct the quadrupole tensor $Q_{ij} = 3x_ix_j - \delta_{ij}r^2$. The eigenvalues of the latter tensor then lead directly to the deformation parameters [9].

Figure 3 shows the evolution of the shape distribution for $^{170}$Dy at inverse temperatures $T^{-1} = 0.5, 1.0, 2.0, \text{ and } 3.0 \text{ MeV}^{-1}$. These contour plots show the free energy $F(\beta, \gamma)$, obtained from the shape probability distribution, $P(\beta, \gamma)$, by

$$F(\beta, \gamma) = -T \ln \frac{\mathcal{F}(\beta, \gamma)}{\beta^3 \sin 3\gamma},$$

where the $\beta^3 \sin 3\gamma$ is the metric in the usual deformation coordinates. As is seen from the plots, deformation clearly sets in with decreasing temperature. At high temperatures, the system is nearly spherical, whereas at lower temperatures, especially at $T^{-1} = 3.0$, there is a prolate minimum on the $\gamma = 0$ axis.

These calculations demonstrate how auxiliary field Monte Carlo methods can be extended to rare earth nuclei. For the first time we have used different major shells for protons and neutrons in such a calculation. We have demonstrated how to obtain canonical information
from grand-canonical sampling, and have introduced a discretization of the field integrals that allows for a much more efficient sampling of the integrand. Results for $^{170}$Dy with a pairing + quadrupole Hamiltonian show qualitatively the expected behavior as a function of both cranking frequency and temperature. While the schematic nature of the Hamiltonian precludes reading too much into our results, such calculations could be used to check various approximation schemes. Furthermore, the recently demonstrated ability to handle more realistic shell-model hamiltonians via Monte Carlo methods [10] should allow these calculations to move beyond the schematic level.

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FIGURES

FIG. 1. Canonical and grand-canonical observables for the uncranked $^{170}$Dy system as a function of $\beta$. Circles represent results of canonical projection of the grand-canonical fields, while squares show the grand-canonical results. Lines are drawn to guide the eye and all error bars are smaller than the symbol sizes. We show expectation values of the energy $\langle H \rangle$, the isoscalar quadrupole moment $\langle Q^2 \rangle$, the valence nucleon number $\langle N \rangle$ and number variance $\langle \Delta N \rangle = \sqrt{\langle N^2 \rangle - \langle N \rangle^2}$ (grand-canonical only), the squared angular momentum $\langle J^2 \rangle$, and $-g\langle P^\dagger P \rangle$, the expectation value of the pairing terms in the hamiltonian.

FIG. 2. Grand-canonical observables for $^{170}$Dy at various cranking frequencies and temperatures. We show the average sign $\langle \Phi \rangle$, the isoscalar quadrupole moment $\langle Q^2 \rangle$, the energy $\langle H \rangle$, the square of the angular momentum $\langle J^2 \rangle$, the moment of inertia $\langle I_2 \rangle$, and the expectation value of the pairing terms in the hamiltonian $-g\langle P^\dagger P \rangle$. Error bars where not shown are approximately the size of the symbols, and lines are drawn to guide the eye.

FIG. 3. Contours of the free energy (as described in the text) in the polar-coordinate $\beta$-$\gamma$ plane for the $^{170}$Dy system. Inverse temperatures are from 0.5 (top) 1.0, 2.0, and 3.0 MeV$^{-1}$ (bottom). Contours are shown at 0.3 MeV intervals, with lighter shades indicating the more probable nuclear shapes. As our calculations become indeterminate at $\gamma = 0$, we have truncated these plots at small $\gamma$. 
TABLES

TABLE I. Physical parameters used in these calculations.

| Orbital   | ε (MeV)      | Orbital   | ε (MeV)      |
|-----------|--------------|-----------|--------------|
| 0g7/2     | −2.24        | 0g9/2     | −3.540       |
| 1d5/2     | −1.979       | 1f7/2     | −3.211       |
| 0h11/2    | −1.120       | 0i13/2    | −2.240       |
| 1d3/2     | −0.122       | 2p3/2     | −1.20        |
| 2s1/2     | 0.000        | 1f5/2     | −0.933       |
|           |              | 2p1/2     | 0.00         |

\( g_p = +0.160 \text{ MeV} \)

\( g_n = +0.131 \text{ MeV} \)

\( \chi = +0.054 \text{ MeV fm}^4 \)