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Final Report: 06-LW-013, Nuclear Physics the Monte Carlo Way

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Abstract

This is document reports the progress and accomplishments achieved in 2006-2007 with LDRD funding under the proposal 06-LW-013, "Nuclear Physics the Monte Carlo Way". The project was a theoretical study to explore a novel approach to dealing with a persistent problem in Monte Carlo approaches to quantum many-body systems. The goal was to implement a solution to the notorious "sign-problem", which if successful, would permit, for the first time, exact solutions to quantum many-body systems that cannot be addressed with other methods.

1. Introduction

In this document, we outline the progress and accomplishments achieved during FY2006-2007with LDRD funding in the proposal 06-LW-013, "Nuclear Physics the Monte Carlo Way". This project was funded under the Lab Wide LDRD competition at Lawrence Livermore National Laboratory. The primary objective of this project was to test the feasibility of implementing a novel approach to solving the generic quantum many-body problem, which is one of the most important problems being addressed in theoretical physics today. Instead of traditional methods based matrix diagonalization, this proposal focused a Monte Carlo method. The principal difficulty with Monte Carlo methods, is the so-called "sign problem". The sign problem, which will discussed in some detail later, is endemic to Monte Carlo approaches to the quantum many-body problem, and is the principal reason that they have not been completely successful in the past. Here, we outline our research in the "shifted-contour method" applied the Auxiliary Field Monte Carlo (AFMC) method

2. Personnel

The team working on the project consisted of:
W. Erich Ormand (PI)
Gergana Stoitcheva (post-doc)
Daniel Neuhauser (UCLA – university collaborator)
David Dean (ORNL – outside collaborator)

During FY2006-2007, funding under the project was used to support Gergana Stoitcheva (100%), the principal post-doctoral researcher on the project and the PI (20%). Additional funds were also procured to support travel for a single collaborative visit to UCLA by the Dr. Stoticheva and to conferences (both Ormand and Stoitcheva) for the purpose of reporting the results to the scientific community.

3. Scientific Motivation

One of the great challenges in physics is to develop a fully microscopic theory for quantum many-body systems that includes the full range of quantum correlations. This problem is ubiquitous in that it spans atomic, condensed matter, and nuclear physics. Traditionally, configuration interaction (CI) methods, which rely on diagonalizing the Hamiltonian, H, within a basis, were used to achieve this goal. But, CI methods are limited in their applicability because typically the basis dimension grows dramatically with particle number. Unfortunately, the near exponential growth in basis dimension outpaces Moore's Law, and dramatically limits the usefulness of CI. One alternative is the Auxiliary-field Monte Carlo (AFMC) method, which was introduced roughly twenty years ago to address large-scale applications of the Hubbard model in condensed-matter physics[1], and to nuclear physics in the 1990's. Since the computational effort

for AFMC scales much more gently with particle number, it seems like a natural approach to large-scale problems. But, AFMC, and other Monte Carlo, methods are often crippled by the notorious Fermonic sign problem, which essentially makes the Monte Carlo sampling impossible. The sign problem substantially limits the efficacy of the AFMC method, and has limited nuclear applications only to even particle systems with simple schematic interactions that were at best semi-realistic.

4. Nuclear Structure Models

The configuration interaction methods are among of the most successful methods for providing accurate and detailed descriptions of electronic structure in atoms and nucleonic degrees of freedom in nuclei. Valence particles are spatially confined to a set of orbitals and influence each other via a residual interaction. A mean-field is often used to provide the basis to build a set states, ϕ_i, that we then use to construct the many-body eigenstates of the nuclear Hamiltonian, i.e., $\Phi_\mu=\Sigma_i\alpha_{\mu i}\phi_i$. Mathematically, the configuration interaction reduces to a matrix-diagonalization problem by computing the matrix elements, $H_{ij}=\langle\phi_i|H|\phi_j\rangle$ between each of the basis states, and then finding the eigenvalues of the resulting matrix. Considerable effort has gone into studying nuclei within this framework (developing effective interactions and operators, etc.), and impressive agreement between theory and experiment has been achieved.

While configuration interaction methods are very powerful, they are really brute-force methods that face substantial computational limitations with increasing particle number. This is dramatically illustrated by the following formulae with enumerates the total number of basis states, N_D, for a two-component system, such atomic nuclei with protons and neutrons,

$$N_D \approx \binom{N_s^p}{N_v^p}\binom{N_s^n}{N_v^n}, \tag{1}$$

where $N_s^{p(n)}$ denotes the number of proton(neutron) single-particle states, and $N_v^{p(n)}$ represents the number of proton (neutron) valence particles. With the deployment of computers such as ATLAS at LLNL and JAGUAR at ORNL it is possible to perform CI calculations for nuclei with basis dimensions, N_D, approaching 10^{10}, which might suffice for basic CI calculations for A~70 nuclei. Pushing to the mass 90-100 region will demand bases of the order 10^{16}. Since the computational effort scales as $N^{1.25}$, we would require a computer 10^6 times more powerful than any platform available today. Indeed, this computational requirement far exceeds even the plans for a future exa-scale computing facility that would likely not be available for the next 10 years. An alternative is to turn to Monte Carlo methods.

5. Monte Carlo Methods

In this section, we describe the basic ideas behind the Auxiliary-Field Monte Carlo Shell Model. This was first applied to the nuclear physics problem in the early 1990's while the PI was a post-doctoral fellow Caltech. More detailed description outlining the method can be found in Refs.[2,3]

We start with the idea that we can "filter" to the ground state energy, E_{GS}, via

$$\lim_{\beta\to\infty}\frac{\langle\varphi_0|e^{-\beta\hat{H}/2}\hat{H}e^{-\beta\hat{H}/2}|\varphi_0\rangle}{\langle\varphi_0|e^{-\beta\hat{H}}|\varphi_0\rangle} = E_{GS}\ , \tag{2}$$

where $\hat{H}$ is the nuclear Hamiltonian, $|\varphi_0\rangle$ is a trial wave function. Because of the similarity to time-evolution in quantum mechanics, the exponential factor $e^{-\beta\hat{H}}$ is called the imaginary-time propagator. Further, we can use the same formalism to describe thermal properties within the canonical ensemble, i.e.,

$$E(\beta) = \frac{Tr\left[\hat{H}e^{-\beta\hat{H}}\right]}{Tr\left[e^{-\beta\hat{H}}\right]}, \tag{3}$$

where $\beta = 1/T$ is the inverse temperature, the denominator is actually the partition function, and the trace of an operator $\hat{O}$ is defined as $Tr\left[\hat{O}\right] = \sum_i \langle \phi_i | \hat{O} | \phi_i \rangle$, with the sum spanning over all the states in the system. Eq. (1) is the basis for the highly successful Green's Function Monte Carlo method that has been applied to ab initio studies of light nuclei. It treats the full Hamiltonian in coordinate space and unfortunately is limited to light nuclei for computational reasons.

At this point, we note that any two-body Hamiltonian can always be expressed as a sum of no more than quadratic operators, namely

$$H = \sum_\alpha \varepsilon_\alpha \hat{O}_\alpha + \frac{1}{2}\sum_\alpha V_\alpha \hat{O}_\alpha^2, \tag{4}$$

where often the operators $\hat{O}_\alpha$ are based on the second-quantized density operators $\hat{\rho}_{ij} = a_i^+ a_j$. The presence of the two-body term in Eq. (3) dramatically increases the complexity in Eq. (2). We can achieve simplification with the Hubbard-Stratonovich (HS) transformation[4], which is really a Gaussian-integral identity, i.e.,

$$e^{\frac{1}{2}\Lambda\hat{O}^2} = \sqrt{\frac{|\Lambda|}{2\pi}} \int d\sigma e^{-\frac{1}{2}|\Lambda|\sigma^2 + s\sigma\Lambda\hat{O}}, \tag{5}$$

where $s = \pm 1$ if $\Lambda \geq 0$ and $s = \pm i$ if $\Lambda < 0$. The imaginary-time propagator in Eqs. (1) and (2) becomes

$$e^{-\beta\hat{H}} = \int D[\sigma] \exp\left[-\tfrac{1}{2}\beta \sum_\alpha |V_\alpha| \sigma_\alpha^2\right] e^{-\beta\hat{h}(\sigma)} \tag{6}$$

where $D[\sigma] = \prod_\alpha \sqrt{\Delta\beta |V_\alpha| / 2\pi}\, d\sigma_\alpha$ and $\hat{h}(\sigma) = \sum_\alpha \left(\varepsilon_\alpha + s_\alpha V_\alpha \sigma_\alpha\right)\hat{O}_\alpha$ is the resultant one-body Hamiltonian. The physical interpretation of $\hat{h}(\sigma)$ is that it represents a constrained mean-field for the system. Indeed, it can be shown that once Eq. (6) is inserted into Eq. (2), the maximum in the integrand corresponds to the so-called Hartree mean field. The power of Eq. (6) is that it substantially simplifies computing observables in Eqs. (2) and (3). Indeed, they can be reduced to determinants of matrices whose dimensions are given by the number of single-particle, N_S, states in the chosen space. This dimension typically ranges in the tens, and maybe a few hundred, and scales much more gently than the total number of many-body states, which typically increases factorially with N_S. The total number of fields needed for the full Hamiltonian is just N_S^2. The final step comes about by noting that the operators $\hat{O}_\alpha$ don't commute so we are forced to "break up" the exponential into N_t time slices via

$$e^{-\beta\hat{H}} = \left(e^{-\Delta\beta\hat{H}}\right)^{N_t} = e^{-\Delta\beta\hat{H}} \cdots e^{-\Delta\beta\hat{H}},$$

with $\Delta\beta = \beta / N_t$. One then performs the HS transformation at each time slice, carefully preserving the time ordering. Finally, Eq. (3) takes the form (for Eq. (2), replace the trace with the matrix element)

$$\left\langle \hat{O} \right\rangle = \frac{\int D[\sigma] \left\langle \hat{O} \right\rangle_\sigma G(\sigma)\xi(\sigma)}{\int D[\sigma] G(\sigma)\xi(\sigma)} \tag{7}$$

where, $G(\sigma)$ is the set of Gaussian factors in Eq. (6), $\xi(\sigma) = Tr\left[e^{-\Delta\beta\hat{h}(\sigma_1)} \cdots e^{-\Delta\beta\hat{h}(\sigma_{N_t})}\right]$ is the trace of the one-body imaginary-time evolution operator, and

$$\left\langle \hat{O} \right\rangle_{\sigma} = \frac{Tr\left[\hat{O}e^{-\Delta\beta\hat{h}(\sigma_1)}\cdots e^{-\Delta\beta\hat{h}(\sigma_1)}\right]}{Tr\left[e^{-\Delta\beta\hat{h}(\sigma_1)}\cdots e^{-\Delta\beta\hat{h}(\sigma_1)}\right]}.$$

The dimension of the integral in Eq. (7) is $N_t \cdot N_S^2$. For an application involving iron nuclei, N_s=20, and typically one needs $N_t \sim 32$, for an integral over 12,800 variables. For so many variables, we turn to Monte Carlo methods. Indeed, Eq. (7) has the typical form of an averaged observable with the weight function $W(\sigma)$, which must be positive definite. We proceed, with $W(\sigma) = G(\sigma)\left|\xi(\sigma)\right|$, and selecting an ensemble $\{\sigma_k\}$ chosen according to $W(\sigma)$. The integrand in Eq. (7) is the average

$$\left\langle \hat{O} \right\rangle_{MC} = \frac{\sum_k \left\langle \hat{O} \right\rangle_{\sigma_k} \Phi(\sigma_k)}{\sum_k \Phi(\sigma_k)}, \tag{8}$$

where $\Phi(\sigma_k) = \xi(\sigma_k)/\left|\xi(\sigma_k)\right|$ is the sign of the weight function, and the error is given by the variance. For a practical application of the method, it is necessary that the sign be at least defined. In general, this is not the case, and often one finds that the denominator in Eq. (7) is very nearly zero. This is generally referred to as the "fermionic sign problem". In early 1990's, we determined the set of conditions under which $W(\sigma)$ would be positive definite[2], and found that only a small class of semi-realistic interactions satisfied this condition and only for an even number of particles. Fully realistic Hamiltonians have bad sign characteristics, and the AFMC method suffered considerable failings when applied to most realistic problems.

The maximum of the weight function is readily found by differentiating $W(\sigma)$ with respect to $\hat{O}_\alpha$ and solving the resulting self-consistent set of equations for each σ_α, i.e,

$$\tilde{\sigma}_\alpha = -s_\alpha \,\mathrm{sgn}(V_\alpha)\left\langle \hat{O}_\alpha \right\rangle_{\sigma}. \tag{9}$$

Depending on the representation of the matrix elements in Eq. (6), Eq. (9) is equivalent to the Hartree mean field value.

Recently[5,6], a modification to the Hamiltonian in Eq. (4) was tried and found to be astonishingly successful in test cases. Instead of the "bare" quadratic operators, one shifts $\hat{O}_\alpha$ by its mean-field, or Hartree, value, i.e., $\hat{O}_\alpha \to \hat{O}_\alpha - \left\langle \hat{O}_\alpha \right\rangle$. Equation (4) becomes

$$H = \sum_\alpha \varepsilon_\alpha \hat{O}_\alpha + \frac{1}{2}\sum_\alpha V_\alpha\left(\hat{O}_\alpha - \left\langle \hat{O}_\alpha \right\rangle\right) + \frac{1}{2}\sum_\alpha V_\alpha\left(2\left\langle \hat{O}_\alpha \right\rangle \hat{O}_\alpha - \left\langle \hat{O}_\alpha \right\rangle^2\right) \tag{10}$$

and in Eq. (6) we apply the HS transformation to the quadratic part $\left(\hat{O}_\alpha - \left\langle \hat{O}_\alpha \right\rangle\right)^2$. The significance of using Eq. (10) is twofold. First, each auxiliary field, σ_α, is shift by $\left\langle \hat{O}_\alpha \right\rangle$ towards the origin, and additional factors are retained in the exponential that suppress negative signs in the weight function. By shifting the fields towards the origin, we have an improved sampling via the Gaussian factor $G(\sigma)$ in Eq. (6) in a rotationally invariant way. This last feature is critical as it preserves important physical quantities that are constants of motion.

6. Other Observables with Monte Carlo Methods

With a successful resolution of the sign problem, several important problems in nuclear physics can be addressed. The method is applicable to finding the ground-state binding energy, and one can make predictions for the mass of very exotic nuclei. Strength functions for electromagnetic and weak transitions can be reliably computed. This is fairly straightforward, as

one uses the AFMC method to compute the imaginary-time correlation of the transition operator $\hat{O}$, namely[2]

$$\left\langle \hat{O}^{+}(\tau)\hat{O}(0)\right\rangle = \left\langle e^{\hat{H}\tau}\hat{O}^{+}e^{-\hat{H}\tau}\hat{O}\right\rangle. \tag{11}$$

Here, we apply the HS transformation to all the imaginary-time propagators and the response function is obtained with the inverse Laplace transform of Eq. (8), which is best evaluated using maximum-entropy reconstruction methods[3]. With the response function of Eq. (8), we can compute electromagnetic and beta-decay strength functions important for astrophysics.

With the thermal energy in Eq. (2), the partition function can be computed via[3]

$$\ln Z(\beta) = \int_{0}^{\beta} d\beta' E(\beta') + \ln Z(0), \tag{12}$$

where $Z(0)$ is just the enumeration of the total number of states in the model space. The density of states is obtained by computing the inverse Laplace transform of $Z(\beta)$, and can be evaluated with either the saddle-point approximation by

$$\rho(E) = \frac{e^{\ln Z+\beta E}}{\sqrt{-2\pi\,\partial E/\partial\beta}} \tag{13}$$

or, again, maximum-entropy reconstruction methods[3]. These microscopic level densities can reduce a primary uncertainty in (n,γ) capture rates important for a proper description of the synthesis of the heavy elements.

Overall, the range of projects that can be addressed with the AFMC method with the sign problem brought under control, is extensive.

7. Connection to High-Performance Computing

The AFMC method as describe here is ideally suited for parallel, high-performance computing, making it an ideal project to for LLNL. Like most Monte Carlo applications, a principal limit is the collection of statistics in order to reduce the estimated uncertainty in the evaluation of Eq. (8). In the simplest applications, the AFMC is what is referred to as embarrassingly parallel as one approach is to perform N_{Proc} independent calculations and simply collect the results after each run. In this mode, the AFMC method achieves high efficiency. As one moves towards more ambitious applications, however, an additional limit will be introduced by the size, N_s, of the model space. In this case, new algorithms that distribute core computations, such as the application of the imaginary-time propagator and the computation of matrix determinants and inverses will need to be implemented.

8. LDRD Accomplishments

Gergana Stoitcheva, who first implemented the shift-contour method for nuclear physics problems[6], was hired as a post-doctoral employee on the project and initiated a collaboration with Prof. Daniel Neuhauser (UCLA) to implement the shifted contour method in a set of codes developed by Stoitcheva. These were independently developed, but broadly based on the code CAMSHAFT developed by the PI and other collaborators (including David Dean) over 15 years ago at Caltech. This effort yielded excellent results for test cases where exact diagonalization methods can be employed. The AFMC calculations were performed with $\Delta\beta = 1/32$ MeV^{-1}. A set of test AFMC calculations were performed by Stoitcheva, which provide a basis for verifying the capability of the shifted-contour method to defeat the sign problem. This is shown in Figs. 1 & 2 for the test cases ^{28}Mg and ^{27}Na, where the thermal energy, $E(\beta)$, and the density of states, $\rho(E)$, compared to exact results. The exact results were obtained by the PI, who used the shell-model

code OXBASH to compute all the 28,503 angular momentum project eigenvalues, E_i, for each nucleus. The thermal energy was then obtained by computing the thermal trace, i.e.,

$$E(\beta) = \frac{\sum_i (2J_i + 1) E_i e^{-\beta E_i}}{\sum_i (2J_i + 1) e^{-\beta E_i}}.$$

The test calculations were performed in the model space defined by $0d_{5/2}$, $0d_{3/2}$, and $1s_{1/2}$ single-particle orbits for both protons and neutrons and the fully realistic Wildenthal interaction[7]. The significance of the ^{27}Na results is that in the past, the sign problem prohibited calculations with an odd number of particles even for the semi-realistic interactions mentioned above.

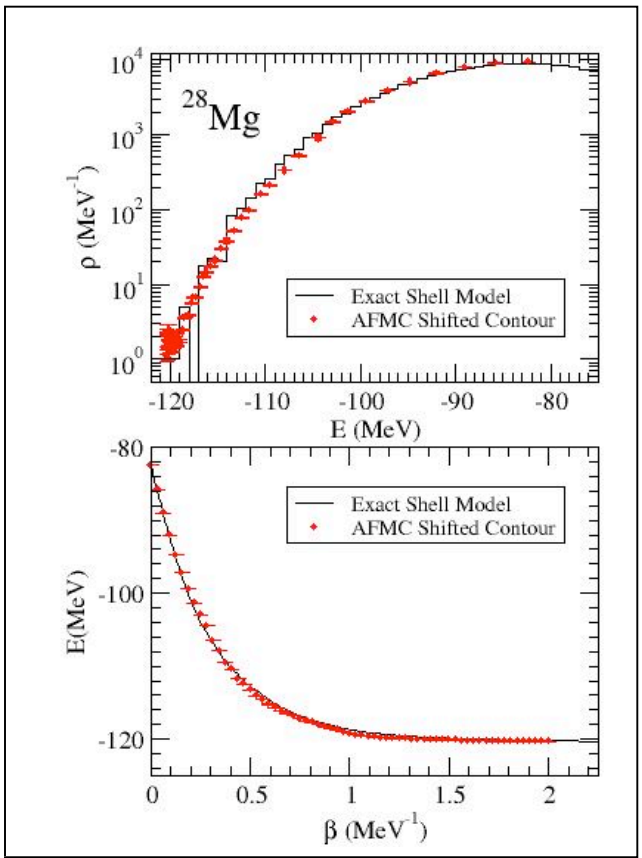

Figure 1. The thermal energy $E(\beta)$ and the density of states $\rho(E)$ for ^{28}Mg calculated with the AFMC method and compared to exact CI results.

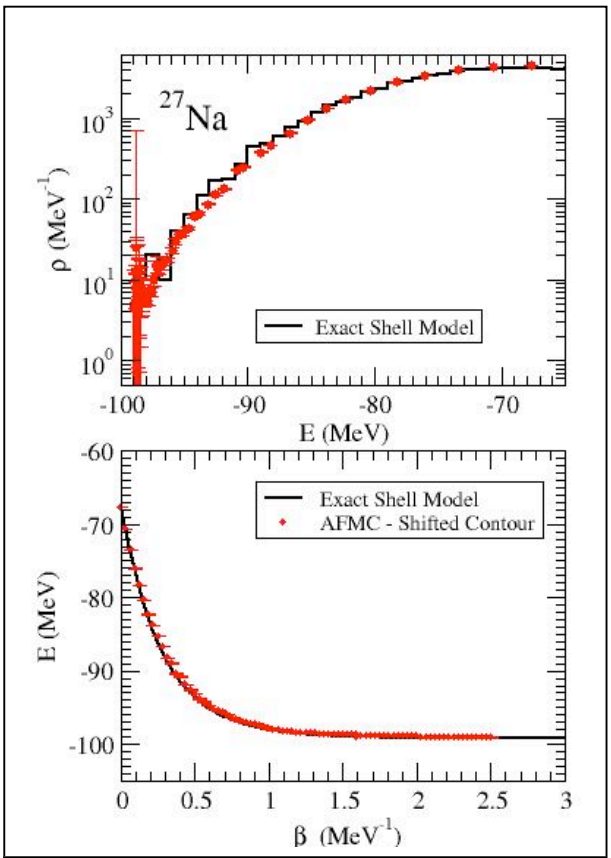

Figure 2. The thermal energy $E(\beta)$ and the density of states $\rho(E)$ for ^{27}Na calculated with the AFMC method and compared to exact CI results.

Shown in Table 1, is a comparison for the calculation of the ground-state energies obtained with OXBASH and the AFMC method in the so-called zero-temperature formalism, i.e., Eq. (2). In general, the AFMC ground-state energies are slightly higher and lie outside of the Monte-Carlo uncertainties. This indicates the need to use a small $\Delta\beta$ value.

Nucleus	CI result (MeV)	AFMC result (MeV)
^{27}Na	-99.230	-99.106(55)
^{28}Mg	-120.532	-120.370(25)

Table 1 Comparison of the AFMC and CI ground-state energies for ^{27}Na and ^{28}Mg

Going beyond test cases, we also applied the method to calculations on a much larger scale within the *fp*-shell, which is defined by $0f_{7/2}$, $0f_{5/2}$, $1p_{3/2}$, and $1p_{1/2}$ single-particle orbits for both protons and neutrons. Calculations for ^{56}Fe, with a dimension $N_D \sim 501\text{M}$, were performed using the GXPF1A interaction[8] using $\Delta\beta = 1/32\,\text{MeV}^{-1}$. With AFMC, we obtained the ground-state energy of -195.687(107) MeV, which compares favorably to the CI result of -195.901 MeV, which was obtained with the shell-model code REDSTICK written by the PI and Calvin Johnson (SDSU). The thermal energy, $E(\beta)$, is shown in the bottom part of Figure 3. In the upper part of Figure 3, the level density, $\rho(E)$, is shown as a function of excitation energy. Unlike, the test cases, it isn't possible to determine the exact shell-model level density. Instead, the level density inferred from experiment is shown[9]. Overall, reasonable agreement with experiment is achieved, with the AFMC result underestimating experiment as the excitation energy increases. This is not unexpected, as at higher excitation energies, we expect levels built on excitations out of the *fp*-shell to enter.

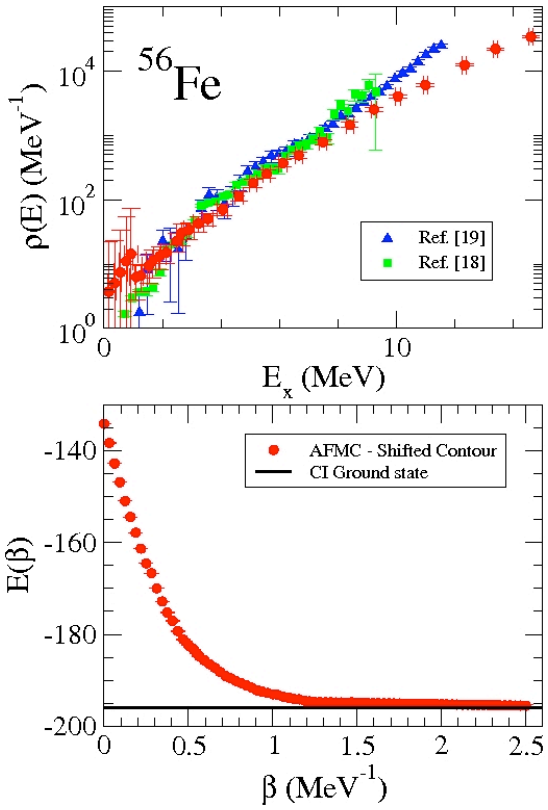

Figure 3. The thermal energy $E(\beta)$ and the density of states $\rho(E)$ for ^{56}Fe calculated with the AFMC method. The solid line in the bottom panel represents the exact CI ground state. In the upper panel, AFMC results are compared with recent experimental data.

9. Research Conclusions and Outlook

While this LDRD funded project came to an end in October 2008, the research team successfully transitioned it from a Lab-wide funded project to an ER-funded project within the PAT Directorate: 08-ERD-018, "Towards a Universal Description of Nuclei with Monte Carlo Methods". The goal was to apply the gains of the new project was to integrate the success of the Lab-wide project into a broader-based effort to develop a more universal picture of atomic nuclei. The main goal was to combine the AFMC method with spherical Hartree-Fock calculations. Here, the Hartree-Fock calculations would be used to provide both the model space and interaction matrix elements to compute the effect of quantum correlations on top of the Hartree-Fock calculation. This would provide for the first time a procedure to move well beyond the simplistic mean-field description most often used for heavy nuclei.

The results presented in the last section were submitted for publication in Physical Review Letters in October 2008 (at the conclusion of this funded LDRD project). The referee reports were fairly positive, and requested more detail on the generic efficacy of the shifted-contour method and some improved calculations, in particular a study of the convergence in the ground-state energy as a function of $\Delta\beta$. In December 2008, our team suffered a substantial setback when Gergana Stoitcheva's laptop suffered a simultaneous motherboard and hard-drive failure. The primary consequence was that all the source codes developed by G. Stoitcheva were lost when we discovered that this laptop was not being backed up by PAT computer support. Consequently, we

were unable to reproduce the previous results. Since the code developed by Stoitcheva was somewhat limited in that it could not compute the imaginary-time autocorrelation functions of Eq. (11), it was a primary goal for the first year of the extended LDRD to implement the shifted-contour method into the existing CAMSHAFT code. Consequently, while this was a setback, we had a recovery plan. Unfortunately, the G. Stoitcheva left the Laboratory and the collaboration in June 2008. While the Pi has coded the shift into CAMSHAFT, it has not been able to reproduce the prior results. Possibly indicating a subtle error in the code. Work is still underway at LLNL to rebuild the codes, in order to apply the AFMC method to a broad range of nuclei. An alternative approach that is a hybrid between the AFMC and CI is also under investigation. In this case, the imaginary-time propagator will be used to generate a set of non-orthogonal basis states (in fact, Slater determinants) to be used in an angular-momentum- and isospin-projected matrix diagonalization. Since the AFMC is based on importance sampling, the action of the imaginary-time propagator will likely generate a subset of important states that can lead to reasonable approximation to the system eigenstates that will be variational and will converge to exact result with a sufficiently large set of states. It is important to note, however, that because the AFMC is importance sampled, and the Slater determinants are deformed this subset should be substantially smaller than the full basis. Some preliminary test-case applications in the *sd*-shell look promising. For example, an AFMC calculation utilizing the shifted contour for ^{24}Mg in the *sd*-shell with the Wildenthal interaction yields an average sign $\langle \Phi \rangle \sim 0.9$ with 1000 Monte Carlo samples using the Metropolis sampling method. The Monte Carlo energy is roughly halfway between the mean-field value and the exact CI result. In addition, the expectation value of the square of the angular momentum is ~7.5, which is substantially lower than the mean-field value of 14.5. Further, previous experience indicated that projecting angular momentum onto just the mean-field solution yielded an energy nearly equivalent to the result obtained in the two time-slice AFMC calculation. Thus, a matrix-diagonalization method based on basis states generated with two or possibly four time slices could be highly promising.

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