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**Statistical Methods for Including Two-Body
Forces in Large System Calculations**

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The difficulty of calculations of properties for large systems of interacting particles is well known. In such systems as nuclei and atoms, we must deal with large numbers of states, often more than 10^8 . The obvious approach to solving such a system would be to calculate the matrix elements of the Hamiltonian (energy operator) between each pair of states and then diagonalize the matrix. Such a method is clearly impossible when dealing with a space of the size of 10^8 or so, because the matrix would then have $(10^8)^2$ or 10^{16} elements. Moreover, even if the computing capability were such as to allow a diagonalization of this size, this would be an impractical solution, since we would then have 10^8 vectors of length 10^3 components for which we would then calculate various averages.

Nearly all of the theoretical work in the field of nuclear level densities has circumvented this problem by making the assumption that the nucleons are non-interacting. The effect of the remaining nucleons on a particular nucleon is approximated by an average potential and one can use statistical mechanics to calculate the level densities.¹ This model is called the Fermi gas model. At a specific thermodynamic temperature θ , the occupancy of a state with energy ϵ_i is postulated to be $1/[e^{(\epsilon_i - \epsilon_f)/\theta} + 1]$ where ϵ_f is the Fermi energy and is determined by the condition that the sum of all the occupancies must equal the total number of nucleons. We then evaluate the grand partition function $\Omega = \sum_i 2n(1 + \exp(-\beta\epsilon_i))$, where $\beta = 1/\theta$ and the sum is over all single particle states. The excitation energy E at the particular value of the temperature chosen will be the sum of the single particle energies times the occupancies for each state and the level density will be the inverse Laplace transform of the partition function:

$$\rho(E) = \frac{1}{(2\pi i)^3} \oint d\beta \oint d\alpha_1 \oint d\alpha_2 e^S, \quad ,$$

where

$$S = \Omega + E/\theta - \frac{\epsilon_{fN}}{\theta} N - \frac{\epsilon_{fZ}}{\theta} Z$$

and where N and Z are the neutron and proton numbers of the nucleus and ϵ_{fN} ($= \alpha N/\beta$) and ϵ_{fZ} ($= \alpha Z/\beta$) are the Fermi energies of the neutron and protons, respectively. Use of the saddle point procedure then relates the level density to the exponential of S (e^S) and certain second derivatives of Ω with respect to the Fermi energies and the thermodynamic temperature.

This procedure is easily coded for a large computer and the equations are quickly evaluated. Unfortunately, there are some fundamental limitations to the formalism. A basic assumption of the model is that the probability that a given state is occupied is independent of whether any other particular state is occupied. We know, of course, that in low-lying nuclear states the nucleons are preferentially paired, i.e. each pair of protons or neutrons couples to 0 angular momentum. In addition, collective states, involving the coherent excitation of many particle-hole pairs each coupled to the same angular momentum, also are prominent in the low-lying spectrum of nuclei. The pairing force can be included by using a super-conducting model for the nucleus; we then have *quasi-particles with modified energies replacing the actual nucleons in our thermodynamic formalism.*¹ It is more difficult to remedy the problem with the collective states and these must normally be added ad hoc to the spectrum. A summary of the difficulties in using the Fermi gas model has recently been presented.²

Although these difficulties are quite serious, lack of an obvious alternative has left the Fermi gas model as the most widely used formalism for calculating nuclear level densities.

Recently, an alternative method for calculating level densities and strength functions has been proposed.³ It is based on the use of the Central Limit Theorem (CLT). This theorem states that the distribution for a statistical

quantity which depends on many variables will tend to a Gaussian distribution in a large space. A general proof of this theorem has never been formulated and, indeed, in some situations the CLT is known to be invalid. One well known example is the case of a system described by an energy matrix which has elements distributed with a Gaussian distribution. For this system, the eigenvalues have not a Gaussian distribution but a semi-circular distribution, i.e., the level density $\rho(E)$ is $C^2 - E^2$, where C is a constant and E is the energy of the system. This system is not particularly realistic, however, since such a matrix corresponds to an N -body Hamiltonian, if there are N particles. Imposing the restriction that the Hamiltonian be two-body results in a matrix which has many zeroes in off-diagonal positions with the remaining matrix elements having a Gaussian distribution. Ironically, changing the matrix element distribution from Gaussian to this modified Gaussian form converts the eigenvalue distribution (level density) to a Gaussian form.

We then need only three parameters to characterize the level density. The Gaussian form is

$$\rho(E) = \frac{N}{\sqrt{2\pi}\sigma} \exp \frac{-(E-E_0)^2}{2\sigma^2}$$

where N is the total number of levels, E_0 is the average energy of all of the levels, $\langle H \rangle$, and $\sigma = [\langle H^2 \rangle - \langle H \rangle^2]^{1/2}$. N is equal to a binomial coefficient giving the number of ways which a specified number of particles can be arranged in a fixed number of orbitals. The difficult task is then to determine the average energy $\langle H \rangle$ and the average square of the energy $\langle H^2 \rangle$ or second moment for all states in the system.

Obviously, if the energy of each state were known, one could simply evaluate directly the quantities $\langle H \rangle$ and $\langle H^2 \rangle$. Since our representation is not diagonal, these individual energy values are not available to us

(without performing a diagonalization). By invoking unitarity, we may evaluate these sums in our non-diagonal basis and know that the result is identical to that in the diagonal representation. Briefly, this is due to the fact that although any one term in the moment (or trace) sum is not simply that due to one actual state of the system, we may include the contributions of a large number of such states by including a large number of basis states in our non-diagonal system. The effect of the two-body force is not to create or destroy states but simply to re-distribute their strength. Thus, by extending our sum over an energy range which is large compared to the strength of two-body forces, these moments may be evaluated in a non-diagonal basis.

There is, however, a further objection to evaluating these sums directly. For a basis with 10^{10} states in it, each sum would involve a lengthy calculation, even on a high-speed computer. Fortunately, the properties of the Hamiltonian allow a much simpler calculational procedure. As previously mentioned, our Hamiltonian is a two-body operator, i.e. all terms in the sum of the contributions for such an operator involve the interaction of no more than two particles. We may then invoke what is called the propagator theorem:³ the expectation value of an n body operator in a specified space is an $n + 1$ term polynomial in the particle number.

The significance of this theorem may be best clarified by an example. Suppose we have a system consisting of 24 mass elements and we wish to calculate the average mass of all systems with m mass elements included. The mass operator $M = \sum_i M_i$ is obviously a one-body operator, so a two-term polynomial would be expected, $M(m) = C_0 + C_1 m$ where m masses are included. Clearly, $M(0) = 0$ and $M(1) = \langle M_i \rangle = \sum_{i=1}^{24} M_i / 24$. For an arbitrary m such that $0 \leq m \leq 24$, we have $M(m) = \langle M_i \rangle m$. Note that for the case where $m = 12$ we would have $\binom{24}{12}$ or 2.7×10^6 separate combinations of 12 mass

elements, but we can find the average value in terms of a sum over 24 mass elements.

Similarly, if we repeat the calculation for the square of the mass M^2 (a two-body operator) we can assert that $M^2 = d_0 + d_1 m + d_2 m^2$.

$$M^2(0) = 0 \text{ so } d_0 = 0. \quad M^2(1) = \frac{\sum M_i^2}{24} \quad \text{and} \quad M^2(2) = \frac{\sum_{i < j} \sum_j M_i M_j}{276} \quad d_1 \text{ and } d_2$$

can be determined by solving the equation for $M^2(m)$ at values of m of 0, 1 and 2 as indicated above. Note that because of the increased complexity of the operator we must now deal with sums over as many as 276 elements (instead of 24 as for $M(m)$), but this number remains much smaller than the 2.7×10^6 terms involved in calculating the average directly for $m = 12$.

An analogous procedure can be used to calculate the expectation values of $\langle H \rangle$ and $\langle H^2 \rangle$. Since H is itself a two-body operator, H^2 will be a four-body operator and this complicates the calculation somewhat. Nonetheless, the calculation of these two moments in spaces as large as 10^{16} has been carried out in less than 1 minute on the CDC 7600 computer.

Some questions remain, however. As previously indicated, no general proof of the central limit theorem is possible, since certain exceptions are known. Can we test the present systems to determine whether they in fact produce a Gaussian distribution for the eigenvalues? Also, can we apply this same technique to the evaluation of other operators, such as gamma-ray strength functions?

A test of the CLT hypothesis for the nuclear and atomic systems of interest here is difficult but possible. If we have available to us moments of the Hamiltonian beyond H^2 (e.g. H^3 , H^4 , etc.) we can verify

that the Gaussian fit obtained gives reasonable values for the higher moments. More generally, we could utilize the higher moments to calculate correction terms to the Gaussian form in an Hermite polynomial expansion for the level density. For a system in which the CLT operates, we should find rapid convergence in such a series, with only the first few terms having a significant effect. One example of such a comparison is shown in Fig. 1. A tabulation of the exact eigenvalues for ^{21}Ne (calculated in a model which allows five active particles and freezes the remaining sixteen into an inert core) is compared with a Gaussian fit and Hermite expansions through the eighth order. Note that the spectrum has a very Gaussian shape, with relatively small corrections provided by the higher moments. It should be pointed out, however, that these corrections are most important for very high and very low regions of the spectrum, and the latter region is the one of most physical interest.

There are also theoretical reasons why we would expect the level distribution to be nearly Gaussian. French⁴ has shown that if a system is characterized by a two-body Hamiltonian, a Gaussian distribution of eigenvalues would be expected. This convergence should actually be enhanced for very large systems where independent tests of the CLT are quite difficult.

It is difficult to assess how difficult the general application of moment techniques to other operators will be. In most cases, use of propagator techniques can easily give second moment results, so the key question is the role played by higher moments for these operators. Because of the interest in higher moments, both for level densities and for other operators, it is important to determine whether such higher

moments can be easily evaluated.

In principle, the propagator technique can be used to obtain higher moments precisely as it has been used to calculate the first two.

Unfortunately, the higher powers of the Hamiltonian (or of any operator) are normally operators of high order. H^3 and H^4 , for example, are six- and eight-body operators, respectively, so the effort to obtain them goes up much beyond that to obtain H and H^2 .

We are presently investigating alternative procedures for evaluating moments in very large spaces. As indicated previously, evaluating the sums for the moments directly is not practical because of the enormous number of terms in each sum. An obvious alternative technique is to choose terms at random from those in the sum and evaluate the sum through Monte Carlo procedures.

The initial tests^{4,5} of this method have been quite promising. A computer code has been developed which allows evaluation of a specified number of the terms in these moment sums for various operators. Let $|\alpha_i\rangle$ denote one of the basis states in our non-diagonal basis. By choosing a number of different i values and calculating the expectation value $\langle \alpha_i | O | \alpha_i \rangle$ for each $|\alpha_i\rangle$ we can estimate the value of the moment of the operator O . In fact it is most efficient to exploit the vector features of modern computers and use as a trial state a so-called random vector:

$$|r_i\rangle = \sum_j \beta_j |\alpha_j\rangle, \text{ where } \sum_j \beta_j^2 = 1 \text{ and } \langle \beta_i \rangle = 0. \text{ Thus, our trial}$$

state is a randomly selected and randomly weighted combination of a number of basis vectors. Use of such r_i with ten to twenty components greatly speeds up the convergence of the moment calculation relative to the use of individual $|\alpha_i\rangle$.

To see this, consider a sample system where our basis vectors are actually eigenvectors. If we choose one vector at random and evaluate $\langle H \rangle$, we will find this quantity H_i has a variance given by $\langle H^2 \rangle - \langle H \rangle^2$. Repeating the calculation N times with different random vectors would reduce the variance by a factor of N . Similarly, making the calculation once for a vector of N components also reduces the variance by a factor of N . Note that there is no explicit dependence of the error on the actual basis size. For a fixed value of $\langle H^2 \rangle - \langle H \rangle^2$, the error in H_i will be the same for one sample vector whether the total basis size is 10^2 or 10^{20} . In fact the larger basis will normally have a larger value of $\langle H^2 \rangle - \langle H \rangle^2$, but the increase is much smaller than the basis size change might suggest. Finally, we note that because our basis states are not eigenstates, there is some built-in averaging, which reduces the variance below the value $\langle H^2 \rangle - \langle H \rangle^2$ even for one basis vector.

We may also speed up the convergence in another way. Suppose we wish to evaluate the first four moments of the Hamiltonian $\langle H \rangle$, $\langle H^2 \rangle$, $\langle H^3 \rangle$ and $\langle H^4 \rangle$. The first and second moments may be calculated easily using propagator techniques. We can use one or both of these moments to "correct" our $|r_i\rangle$ vectors to have the proper values of $\langle H \rangle$ or $\langle H^2 \rangle$. We then would expect better convergence for the values of $\langle H^3 \rangle$ and $\langle H^4 \rangle$ when using a set $|r'_i\rangle$ of random vectors, each of which is adjusted to produce exactly correct values of $\langle H \rangle$ and $\langle H^2 \rangle$. Preliminary tests⁴ of this technique have been quite promising.

During the next year we plan to utilize this procedure to calculate nuclear level densities for a number of light ($A \sim 30$) and medium mass ($A \sim 90$) nuclei. In addition to information about the level densities

we anticipate developing a better understanding of the energy dependence of gamma-ray strength functions. A group at Los Alamos is utilizing these techniques to calculate atomic level densities and has made considerable progress.

In the longer term moment techniques can be used to improve our understanding of basis truncation effects. Shell model calculations to this point have been limited to rather small bases and in most cases the two-body matrix elements have had to be "renormalized," that is, adjustments in the values of these matrix elements have been made to achieve fits to experimental data. This is probably due to the fact that small parts of the real wave function come from parts of the basis that have not been included in the calculation. Comparisons between small basis and large basis calculations (the latter to be made with moment methods) should help determine whether the renormalization is due entirely to the limited basis size. If not, we may be able to pinpoint deficiencies in our present parameterizations of the nuclear force.

References

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Figure Caption

Fig. 1. Distribution of level energies in the nucleus ^{21}Ne calculated with the assumptions explained in the text. Calculated points are indicated by Δ , and the Gaussian and eighth order Hermite polynomial fits are indicated with (—) and ($\cdot$ —), respectively. Note the close agreement with the Gaussian form.

FIGURE 1