TUNNELING OF A MANY-FERMION SYSTEM IN ONE DIMENSION

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ABSTRACT

A method is presented for stochastic evaluation of ground state properties and tunneling decay of many-fermion systems in one spatial dimension. Application to a model problem defined to produce saturation, strong short-range repulsive-core correlations, and spontaneous fission provides the opportunity to test the stationary-phase approximation and assumptions concerning the effective interaction presently utilized in the mean-field theory of spontaneous fission.

I. INTRODUCTION

Since the first application to the nuclear many-body problem at the Saclay TDHF workshop three years ago, significant progress has been made in developing functional integral techniques for nuclear physics.[1] Despite new insight provided by alternative formulations of functional integral representations of the evolution operator, fuller understanding of the freedom in defining the mean field, and experience obtained from a variety of applications, two crucial, fundamental questions still remain unanswered: What is the validity of the stationary-phase approximation (SPA) and how does one define an appropriate effective interaction to use in the resulting mean-field equations? These questions are obviously interrelated and would be resolved simultaneously by a fundamental treatment of many-body correlations.

In the absence of a practical general theory for correlations, it would be of significant value to test both the SPA and the treatment of the effective interaction by comparison with the exact solution for a model which incorporates the essential features of the nuclear many-body problem. Thus, in this work, Monte Carlo techniques will be described for the exact evaluation, subject only to controllable statistical sampling errors, of functional integrals specifying ground state observables and tunneling decay of many-fermion systems. Much of this work is based upon the approach to Monte Carlo developed by S. Koonin[3] and extensive discussions with H. Orland and the application to tunneling is being pursued in collaboration with G. Bertsch.

Given that one of the primary objectives is accurate treatment of many-body correlations, I have chosen to utilize a coordinate-space path integral representation which is well-suited to forces with strongly repulsive cores. Unfortunately, as will become evident subsequently, Monte Carlo techniques for such path integrals are presently only practical in one spatial dimension, so this convenience in treating repulsive cores comes at a high price. Nevertheless, it is instructive to begin with a simple, well-controlled problem and I believe there is considerable relevant many-body physics to be learned in one-dimension. Furthermore, there is reason to hope that the use of

Monte Carlo evaluation of other functional integral representations, such as the auxiliary field described at this meeting by Steve Koonin, or the Monte Carlo methods of Kalos or Zabolitzky may ultimately allow one to extend the present investigation to higher dimensions.

II. QUANTUM MECHANICS FOR ONE PARTICLE IN A POTENTIAL WELL

It is useful to tersely review the fundamental functional integral for the quantum mechanics of a single particle, and its evaluation by the SPA and Monte Carlo methods. The real-time evolution operator may be evaluated by dividing the time continuum into discrete steps of size ε, inserting complete sets of position space and momentum space eigenstates at each step, replacing $\hat{x}$ and $\hat{p}$ by their eigenvalues and integrating out the momenta to obtain[2]

$$\langle x_{N+1}|e^{-iHT}|x_0\rangle = \int (x_1 \cdots x_N)\, e^{i\varepsilon \sum_n \left[\frac{m}{2}\left(\frac{x_{n+1}-x_n}{\varepsilon}\right)^2 - V(x_n)\right]} \tag{1}$$

The exponent is recognized as a discrete approximation to the classical action $S(x)$.

A) The Stationary Phase Approximation

To calculate eigenstates of H it is convenient to evaluate the Fourier transform of the trace of the evolution operator:

$$\begin{aligned} i\int_0^\infty dT e^{iET} \mathrm{tr}\, e^{-HT} &= \sum_n \frac{\langle n|\ |n\rangle}{E_n - E - i\eta} \\ &= i\int dT e^{iET} \int d\bar{q} \int \mathcal{D}[q(t)] e^{iS[q(t)]}\Big|_{q(T)=q(0)=\bar{q}} \end{aligned} \tag{2}$$

For a particle in a single well, sequential application of the SPA to the three integrals yields a sum over all periodic classical trajectories in the well with energy E, and the resulting geometric series yields poles when the Bohr-Sommerfeld quantization condition is satisfied. Corrections to the lowest SPA systematically sum the fluctuations of the coordinates about the classical trajectory at each time step. For the double well the new feature arises that trajectories with imaginary time provide the leading SPA contribution in classically forbidden regions, corresponding to classical motion in the inverted potential. Summation of the multiple geometric series of all classical trajectories in the three allowed and forbidden regions yields an expression for the level density for which a WKB formula for the level splitting between the two lowest eigenstates of a degenerate well or the lifetime of a metastable state may be calculated. In the case of a double well with a high barrier, the classical solution may be picturesquely visualized in terms of instantons, classical solutions in the inverted well connecting arbitrary numbers of periodic solutions in the two classically allowed wells. Corrections to the SPA again build up all the fluctuations about these classical paths required to obtain the full quantum mechanics of the exact functional integral.

B) Monte Carlo Evaluation of Functional Integrals

An integral with an integrand expressed as the product of a function f(x) times a probability distribution P(x) may be evaluated stochastically

$$\int f(x)\, P(x) = \lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} f(x_i) \tag{3}$$

where the x_i's are randomly distributed according to the distribution P(x). Although this formula is very general, it is only useful when the variance may be made sufficiently small, which in practice requires that the integrand be positive or at least dominantly positive. This requirement forces one to deal with the Euclidean, or imaginary time, evolution operator to eliminate cancelling phases with the corollary that the exponential weighting of eigenstates restricts practical calculations to low-lying states. Nearly cancelling positive and negative contributions arising from antisymmetry pose additional problems for fermions which will be apparent below.

Even when one has selected a functional integral representation for the evolution operator, considerable freedom exists in the choice of the physical quantity to be calculated. The fundamental trade-off is building into the calculation as much of the physics of the solution as one understands a priori versus unduely prejudicing the results by misconceptions.

1) Initial Value Form

A physically transparent way to formulate a random walk for the ground state introduced by Koonin[3] is to use the imaginary-time counterpart of eq.(1) to generate a population of points distributed according to $\Psi(x)$. The matrix element

$$\begin{aligned} \langle \Phi_2 | e^{-\beta(H-E)} | \Phi_1 \rangle = \int dx_1 \ldots dx_N \, \langle \Phi_2 | x_N \rangle \langle x_N | e^{-\varepsilon(H-E)} | x_{N-1} \rangle \times \\ \times \; \langle x_{N-1} | e^{-\varepsilon(H-E)} \ldots | x_2 \rangle \langle x_2 | e^{-\varepsilon(H-E)} | x_1 \rangle \langle x_1 | \Phi_1 \rangle \end{aligned} \tag{4}$$

may be evaluated as a multidimensional integral using the Monte Carlo method as follows, where for the moment E should be regarded as an arbitrary constant. An ensemble of points $\{x_1\}$ is selected with probability distribution $\phi(x_1)$ (which is necessarily assumed positive). For each x_{n-1}, x_n is generated according to the distribution

$$\langle x_n | e^{-\varepsilon(H-E)} | x_{n-1} \rangle = \frac{2m\pi}{\varepsilon} e^{-\frac{m}{2\varepsilon}(x_n - x_{n-1})^2 - (\frac{V(x_n)+V(x_{n-1})}{2} - E)\varepsilon} \tag{5}$$

The kinetic energy alone, represented by the gaussian factor, would distribute x_n within in a region of the order $\sqrt{\varepsilon}$ of x_{n-1}, leading to the physical spreading of a free wave packet. Depending upon whether V-E is positive or negative, the distribution is normalized less than or greater than one, resulting in the deletion of points in classically forbidden regions and the replication of points where the potential is most attractive. Finally the matrix element in eq.(4) is calculated by evaluating $\phi_2(x_N)$ for the ensemble of values $\{x_N\}$ as in eq.(3).

The ground state energy may be calculated two ways. Evaluating the ratio of two matrix elements of the form of eq.(4) yields the trial energy

$$E_0 = \lim_{\beta\to\infty} \frac{\langle H\Phi | e^{-\beta(H-E)} | \phi\rangle}{\langle \Phi | e^{-\beta(H-E)} | \phi\rangle} \tag{6}$$

In practice, once β is sufficiently large one can generate independent populations of $\{x\}$ distributed according to the ground state wave function by continuing iteration of eq.(5) and thereby improve statistics to any required accuracy. Thus far E has been an arbitrary parameter which controls the overall growth or decrease of the population $\{x\}$. The value of E which keeps the population stable provides an independent determination of the ground state energy which will be denoted here as the normalization energy.

Importance sampling may be introduced to decrease the variance of observables of interest.[4] Essentially, one writes the evolution operator for $\phi(x)\psi(x)$ rather than $\psi(x)$ by multiplying and dividing by a physically motivated trial function $\phi(x)$ at each step. For example, the numerator of eq.(5) is evaluated

$$\langle \Phi | He^{-\beta(H-E)} | \phi\rangle = \int dx_1 \ldots dx_N \langle \Phi | H\frac{1}{\phi} | x_N\rangle \times \\ \times \langle x_N | \phi e^{-\varepsilon(H-E)} \frac{1}{\phi} | x_{N-1}\rangle \ldots \langle x_2 | \phi e^{-\varepsilon(H-E)} \frac{1}{\phi} | x_1\rangle \langle x_1 | \phi | \Phi\rangle \tag{7}$$

where

$$\langle x_n | \phi e^{-\varepsilon(H-E)} \frac{1}{\phi} | x_{n-1}\rangle \\ = \sqrt{\frac{2m\pi}{\varepsilon}}\; e^{-\frac{m}{2\varepsilon}\left(x_n - x_{n-1} - \varepsilon \frac{\frac{\partial}{\partial x}\phi(x_{n-1})}{m\,\phi(x_{n-1})}\right)^2 - \varepsilon\frac{(H-E)\phi(x_{n-1})}{\phi(x_{n-1})}} \tag{8}$$

Evolution of random walks using eq.(8) differs from eq.(5) in two respects. The gaussian is now shifted by a drift term proportional to ϕ'/ϕ which improves statistics by moving points toward regions where the wave function is largest and points are added and deleted only to the extent to which $H\phi$ differs from $E\phi$. If $\phi(x)$ were the ground state wave function, the energy estimate would be exact and in practice a reasonable trial function significantly increases the accuracy of the Monte Carlo approximation.

Whereas the initial value form offers the advantage of utilizing physical insight in the selection of $|\Phi\rangle$ to obtain an excellent approximation to the energy, other observables are either inconvenient to calculate or require the introduction of additional approximations. The energy splitting of the two lowest eigenstates in a double well, and thus the penetrability of a potential barrier, may be approximately calculated by the following method.[5] Let ψ_L and ψ_R denote approximate eigenstates localized in the left and right wells respectively. To within errors which are exponentially small for a high barrier, the two lowest eigenstates are $\psi_+ \sim \frac{1}{\sqrt{2}}(\psi_L + \psi_R)$ with energy E_0 and

$\psi_- \sim -\frac{1}{\sqrt{2}}(\psi_L - \psi_R)$, with energy E_0+2V, where $V = \langle\psi_L|H|\psi_R\rangle$ and the next eigenstate is separated by energy $\Delta>>2V$. Taking $\beta>>\frac{1}{\Delta}$, the expansion for $e^{-\beta(H-E_0)}$ may be approximated by the lowest two terms

$$e^{-\beta(H-E_0)} \approx |\psi_+\rangle\langle\psi_+| + |\psi_-\rangle\, e^{-2V\beta}\langle\psi_-| + \mathcal{O}e^{-\beta\Delta} \tag{9}$$

so that defining trial functions Φ_L and Φ_R localized in the left and right wells respectively

$$\frac{\langle\Phi_L|e^{-\beta(H-E_0)}|\Phi_R\rangle}{[\langle\Phi_L|e^{-\beta(H-E_0)}|\Phi_L\rangle\langle\Phi_R|e^{-\beta(H-E_0)}|\Phi_R\rangle]^{1/2}} \approx \frac{\langle\Phi_L|\psi_L\rangle\langle\Phi_R|\psi_R\rangle}{[|\langle\Phi_L|\psi_L\rangle|^2|\langle\Phi_R|\psi_R\rangle|^2]^{1/2}} \quad \frac{(1-e^{-2V\beta})}{(1+e^{-2V\beta})} = \tanh(V\beta) \tag{10}$$

independent of these trial functions. If one wishes to calculate the lifetime of a metastable state, one may do so by erecting a barrier to convert the potential into a degenerate double well, calculating the matrix element V, and applying the Fermi golden rule with the calculated final density of states. Although this latter procedure has been checked for a representative test case[5], all the relevant physics of barrier penetration is already contained in the splitting of the double well, and we shall henceforth use this quantity to test the validity of the SPA and the effective interaction.

2) Evaluation of Trace

A convenient method for the evaluation of ground state expectation values of operators is calculation of an appropriate trace. A local one-body operator, for example, may be calculated as follows

$$\langle 0|\mathcal{O}|0\rangle = \lim_{\beta\to\infty}\frac{\sum_\alpha \langle\alpha|\mathcal{O}|\alpha\rangle e^{-\beta E_\alpha}}{\sum_\alpha e^{-\beta E_\alpha}} = \lim_{\beta\to\infty}\frac{\mathrm{Tr}\,\mathcal{O}e^{-\beta H}}{\mathrm{Tr}\,e^{-\beta H}} \tag{11a}$$

$$= \lim_{\beta\to\infty}\frac{\int dx\langle x|\mathcal{O}e^{-\beta H}|x\rangle}{\int dx\langle x|e^{-\beta H}|x\rangle} = \lim_{N\to\infty}\int dx_1\ldots dx_N\Big(\sum_{s=1}^{N}\frac{\mathcal{O}(x_s)}{N}\Big)\frac{e^{-S(x_1\ldots x_N)}}{\int dx_1\ldots dx_N\, e^{-S(x_1\ldots x_N)}}$$

$$= \lim_{N\to\infty}\frac{1}{M}\sum_{i=1}^{M}\frac{1}{N}\sum_{s=1}^{N}\mathcal{O}(x_s^{(i)})$$

where the action is given by

$$S(x_1\ldots x_N) = \sum_{n=1}^{N}\Big[\frac{m}{2\varepsilon}(x_{n+1}-x_n)^2 + \varepsilon V(x_n)\Big] \tag{11b}$$

with the periodic condition $x_{N+1} = x_1$ or by the corresponding importance sampled expression in eq.(8) and $\{x_s^{(i)}\}$ denotes the i^{th} set of variables $x_1\ldots x_N$ distributed according

to the probability distribution

$$P = \frac{e^{-S(x_1 \ldots x_N)}}{\int dx_1 \ldots dx_N \, e^{-S(x_1 \ldots x_N)}} \tag{11c}$$

Note that since $\mathcal{O}$ may be evaluated at any time step, statistical errors have been minimized in eq.(11) by averaging over all times.

Evaluation of non-local operators such as the kinetic energy is somewhat more difficult. Placing $\frac{p^2}{2m}$ at the n^{th} time step in the imaginary time counterpart to eq.(1) yields the results

$$\langle T \rangle = \frac{1}{M} \sum_{i=1}^{M} \sum_{n} -\frac{m}{2} \frac{(x_{n+1}^{(i)} - x_n^{(i)})(x_n^{(i)} - x_{n-1}^{(i)})}{\varepsilon^2} \tag{12a}$$

or

$$T = \frac{1}{M} \sum_{i=1}^{M} \sum_{n} \left(\frac{1}{2\varepsilon} - \frac{m}{2} \frac{(x_n^{(i)} - x_{n-1}^{(i)})^2}{\varepsilon^2}\right) \tag{12b}$$

depending upon whether the two p's are grouped with adjacent steps or both p's are associated with the same step. Equation (12b) is particularly unsuitable since the $\frac{1}{\varepsilon}$ singularity in the first term must be cancelled numerically by the second, but even the alternative (12a) is generally not sufficiently accurate. Hence, it is convenient to use the virial theorem,

$$\langle T \rangle = \frac{1}{2} \langle x V'(x) \rangle \tag{12c}$$

and to evaluate the ground state energy by calculating the expectation value of the local operator $\tilde{V}(x)=V(x) + \frac{1}{2}xV'(x)$. The only practical disadvantage of this method is that step function potentials and potentials with more than one infinite barrier cannot be treated at all and potentials with very large gradients may yield undesirably large variance.

The energy of the first excited state, and in particular the splitting in a double well, may be calculated by evaluating the correlation function

$$\Gamma(\tau) = \frac{\mathrm{tr}\, \mathcal{O}(t+\tau)\mathcal{O}(t)e^{-\beta H}}{\mathrm{tr}\, e^{-\beta H}} = \frac{1}{MN} \sum_{i=1}^{M} \sum_{s=1}^{N} \mathcal{O}(x_s^{(i)}) \, \mathcal{O}(x_{s+r}^{(i)}) \tag{13}$$

where $\tau = r\varepsilon$, s+r is defined mod N by periodicity, and $\{x_s^{(i)}\}$ is distributed as before according to eq.(12). If $\beta \gg \tau \gg \Delta$, where Δ is the energy of the second excited state as before, then

$$\frac{\mathrm{tr}\, \mathcal{O}(t+\tau)\, \mathcal{O}(t)e^{-\beta H}}{\mathrm{tr}\, e^{-\beta H}} = \frac{\sum_{\alpha} \langle\alpha|\mathcal{O}|\gamma\rangle\langle\gamma|\mathcal{O}|\alpha\rangle \, e^{-E_\alpha \beta} \, e^{-(E_\gamma - E_\alpha)\tau}}{\sum_{\alpha} e^{-E_\alpha \beta}}$$
$$\to \sum_{\gamma} e^{-(E_\gamma - E_0)\tau} |\langle 0|\mathcal{O}|\gamma\rangle|^2 \qquad \to e^{-(E_1 - E_0)\tau} |\langle 0|\mathcal{O}|1\rangle|^2 - |\langle 0|\mathcal{O}|0\rangle|^2 \tag{14}$$

and the splitting (E_1-E_0) may be determined by the decay of the correlation function.

Exact evaluation of operators of interest thus reduces to the problem of sampling the distribution P in eq.(12), which may be accomplished by means of the Metropolis algorithm.[6] Considering first the case of a single variable, a Markov random walk to generate a population distributed according to $e^{-S(x)}$ may be generated as follows. Given a value $x^{(i)}$, a new value $x^{(i+1)}$ is defined by selecting a tentative value x_t distributed about $x^{(i)}$ according to a function $f(|x_t-x^{(i)}|)$ and accepting or rejecting this tentative choice on the basis of the change in action, $\Delta S = S(x_t)-S(x^{(i)})$. Specifically, the algorithm proceeds by the following three steps:

a) Define

$$x_t = x^{(i)} + \xi\Delta x \tag{15}$$

where ξ is a random variable uniformly distributed on the interval $[-1/2,1/2]$ and Δx is a parameter selected to optimize convergence by yielding an acceptance ratio of the order of 50%. Thus, f(x) is $\theta(\Delta x/2 - |x|)$.

b) If $S(x_t) \leq S(x^{(i)})$, then $x^{(i+1)} = x_t$.

c) If $S(x_t) > S(x^{(i)})$, select a random variable η uniformly distributed on the unit interval [0,1]

$$\text{If } e^{-[S(x_t)-S(x^{(i)})]} > \eta, \text{ then } x^{(i+1)} = x_t$$
$$\text{If } e^{-[S(x_t)-S(x^{(i)})]} \leq \eta, \text{ then } x^{(i+1)} = x^{(i)}$$

Thus, if the action is decreased, the tentative value is accepted. If the action is increased, the tentative value is accepted with probability $e^{-\Delta S}$ and rejected otherwise.

It is simple to verify that $e^{-S(x)}$ is an equilibrium solution to the random walk defined by this rule. Consider the probabilities that $x\to y$ and that $y\to x$. In the case $S(y) < S(x)$, straightforward application of the rule yields the ratio

$$\frac{P(x\to y)}{P(y\to x)} = \frac{f(|x-y|)}{f(|y-x|)} \quad \frac{1}{e^{-[S(x)-S(y)]}} = \frac{e^{-S(y)}}{e^{-S(x)}} \tag{16}$$

The same ratio is obtained for the case $S(x) < S(y)$ so that summing over all x and using the fact $\sum_x P(y\to x) = 1$,

$$\sum_x e^{-S(x)} P(x\to y) = \sum_x e^{-S(y)} P(y\to x) = e^{-S(y)} \tag{17}$$

Thus, the rule evolves the distribution $e^{-S(x)}$ into itself so it is indeed an equilibrium solution.

Generalization to distributions of many variables is straightforward. One may sweep through the time lattice varying each x_n independently in turn, and accepting or

rejecting the tentative change on the basis of $\Delta S = S(x_1^{(i)}\ldots x_{n-1}^{(i)}, x_t, x_{n+1}^{(i)}\ldots x_N^{(i)}) - S(x_1^{(i)}\ldots x_N^{(i)})$. Since each step in the sweep satisfies the microreversibility condition eq. (16), $e^{S(x_1\ldots x_N)}$ is an equilibrium solution as before. For subsequent application to collective motion, it is useful to note that the argument also applies to variation of any combination of the x's as well. The question of convergence of the random walk is much more complicated. An especially simple proof may be constructed in the special case that each step has a non-vanishing probability for reaching every configuration[7] and a proof for the method described here can be constructed using the Perron-Frobenius Theorem.[8]

A pedagogical application of the Metropolis method to the calculation of the trace for the harmonic and anharmonic oscillators is given by Creutz and Freedman.[7] A particularly instructive result is the graph of a typical trajectory in a double well in which one clearly observes random fluctuations about the classical solutions in the minimum in each well connected by instanton-like paths in the classically forbidden region.

III. THE MANY-FERMION PROBLEM.

A number of alternative functional integral representations exist for many-fermion systems, including the many-particle generalization of the path integral, eq. (1), an integral over an auxiliary field, and integrals over overcomplete sets of boson coherent states, determinants, and Grassman variables. These formulations thus offer a number of different possibilities for application of the SPA and Monte Carlo techniques.

A) SPA Bounce Equations

Application of the SPA to the many-particle Feynman path integral yields classical equations of motion which are not a particularly useful starting point for the nuclear many-body problem. All the remaining formulations yield similar equations at the SPA level, corresponding to self-consistent Hartree Fock(or in some cases Hartree) equations in real or imaginary time for solutions in classically allowed or forbidden regions respectively.[1] Including exchange terms for convenience, the bounce equation for spontaneous fission is

$$\left[-\frac{\partial}{\partial\tau} + \frac{1}{2m}\nabla^2 - \int dr' v(r-r')\sum_k \phi_k^c(r',-\tau)\phi_k^c(r',\tau)\right]\phi_\ell^c(r,\tau) = -\frac{\alpha_\ell^c}{\hbar}\phi_\ell^c(r,\tau) \qquad (18a)$$

yielding a total width equal to the sum over partial widths for each distinct solution $\{\phi_i^c\}$ to eq.(18a)

$$\Gamma = \sum_c K^c e^{-\int d\tau dr \sum_k \phi_k^c(r,-\tau)\frac{\partial}{\partial\tau}\phi_k^c(r,\tau)} \qquad (18b)$$

The salient uncertainties in this result discussed in the introduction are the absence of an explicit small parameter for the SPA and the justification for replacing the bare interaction by an effective interaction.

B) Monte Carlo Solution of the Many-Fermion Problem

The alternative functional integral representations of the many-fermion evolution operator discussed above also yield significantly different Monte Carlo problems. In the Feynman path integral, the number of stochastic variables equals the number of particles. All the other forms involve fields which must be defined on a spatial mesh and hence necessarily involve many more variables than particles. In the model problem discussed subsequently for example, one needs on the order of 20 mesh points in an interval occupied by a single particle for adequate accuracy, as well as many additional points at the edge of the nucleus to generate the exponential tail of the wave function, so even a ten-particle problem in one dimension involves over 200 degrees of freedom. A comparable problem in three dimensions involves 10^7 degrees of freedom rendering the study of hard core potentials impractical with present computers.

A second crucial consideration is the necessity of casting the integrand of the integral to be performed by Monte Carlo sampling into non-negative or at least dominantly positive form. This appears to be possible for the auxiliary field form in three dimensions, whereas at present no corresponding coordinate-space form has been developed which is suitable in more than one dimension.

Insertion of a complete set of antisymmetrized many-particle states $|x_1 \ldots x_A\rangle$ at each time step yields the following generalization of eq.(5) for the matrix element of the evolution operator for infinitesimal time ε

$$
\begin{aligned}
&\langle x_1^{\,n} \ldots x_A^{\,n} | e^{-\varepsilon(H-E)} | x_1^{\,n-1} \ldots x_A^{\,n-1} \rangle \\
&\quad = \sum_P \varepsilon^P \, e^{-\frac{m}{2\varepsilon} \sum_i (x_{Pi}^n - x_i^{n-1})^2 - \varepsilon\{\frac{1}{4} \sum_{ij} [v(|x_i^{n-1} - x_j^{n-1}|) + v(|x_i^n - x_j^n|)] - E\}} \\
&\quad = e^{-\frac{m}{2\varepsilon} \sum_i (x_i^n - x_i^{n-1})^2} \det \left| e^{-\frac{m}{2\varepsilon}[(x_i^n - x_j^{n-1})^2 - (x_i^n - x_i^{n-1})^2}\right| \times \\
&\quad \times e^{-\varepsilon\{\frac{1}{4} \sum_{ij} [v(|x_i^{n-1} - x_j^{n-1}|) + v(|x_i^n - x_j^n|)] - E\}}
\end{aligned}
\tag{19}
$$

where the superscript on x denotes the time and the subscript indicates the particle. In one dimension, the signs in eq.(19) are totally innocuous. The sign of the matrix element at each step arising from the determinant is just the sign of the permutation required to bring the x^n's into the same order as the x^{n-1}'s. Hence the cummulative sign after any number of steps is path-independent and is the sign of the permutation required to make the final order equal to the initial order. It does not affect matrix elements of the evolution operator with antisymmetrized states or the trace of the evolution operator times a symmetric operator.

In higher dimension the sign is path-dependent. Two particles may interchange in a single step, generating a minus sign, or circle around each other by a series of small steps, each corresponding to a positive matrix element. The net result is nearly complete cancellation of positive and negative contributions from which it becomes ex-

ceedingly difficult to extract statistically significant information for large β.

For Monte Carlo calculations in one-dimension, it is convenient to work in the subspace $x_1 < x_2 < x_3 \ldots < x_A$. The determinant in eq.(19) already yields zero when any two coordinates are equal, and one in addition simply includes θ-functions forbidding all interchanges. Physically, this is equivalent to assuming an infinite potential at all boundaries $x_i = x_j$ which generates the nodes required by antisymmetry. In this domain the determinant may be replaced by the following product in the limit $\varepsilon \to 0$:

$$\det \left| e^{-\frac{m}{2\varepsilon}\left[(x_i^n - x_j^{n-1})^2 - (x_i^n - x_i^{n-1})^2\right]} \right| \underset{\varepsilon\to 0}{\longrightarrow} \prod_{i=2}^{A} \left(1 - e^{-\frac{m}{\varepsilon}(x_i^n - x_{i-1}^n)(x_i^{n-1} - x_{i-1}^{n-1})}\right) \tag{20}$$

yielding an action which may be sampled efficiently. As in the single-particle case, importance sampling may be introduced by multiplying and dividing by a trial function $\phi(x_1 \ldots x_A)$ and eq.(19) is replaced by

$$\langle x_1^n \ldots x_A^n | \phi e^{-\varepsilon(H-E)} \frac{1}{\phi} | x_1^{n-1} \ldots x_A^{n-1} \rangle = \sum_P \varepsilon^P e^{-\frac{m}{2\varepsilon}\sum_i \left(x_{Pi}^n - x_i^{n-1} - \frac{\varepsilon \frac{\partial}{\partial x_i^{n-1}} \phi(x_1^{n-1} \ldots x_A^{n-1})}{\phi(x_1^{n-1} \ldots x_A^{n-1})} \right)^2} \tag{21}$$

A convenient form of trial function, both for importance sampling and for the matrix elements arising in the initial value form, is the following

$$\phi(x_1 \ldots x_n) = \prod_{i<j} g(x_i - x_j) \prod_k f(x_k) \tag{22}$$

where g is odd and asymptotically approaches ± 1 and f localizes the density properly. Note this ansatz is different from the usual Jastrow form since the antisymmetry is included in the two-body rather than one-body component. Nuclear matter is calculated by placing A particles in a box of length L with periodic boundary conditions. For this case $g(x) = \sin(\frac{x}{L})$ and $f(x) = 1$ which provides an efficient means of representing a Slater determinant. For finite nuclei $g(x) = \tanh(bx)$, f(x) is a fermi function, and the parameters are adjusted to produce a reasonable density and two-body correlation function.

Thus far, the discussion has tacitly assumed a single spin state. For spin-independent forces and spin degeneracy M, the ground state energy and spin-independent observables may be calculated by including determinatal factors and forbidding interchanges only within each of the ordered subsets $\{x_1 \ldots x_{\frac{A}{M}}\}$, $\{x_{\frac{A}{M}+1} \ldots x_{\frac{2A}{M}}\}$, $\ldots \{x_{\frac{(M-1)A}{M}} \ldots x_A\}$. When the spin degeneracy, M, equals the number of particles, A, one obtains the boson ground state.

In order to convert the fission problem into a double-well problem, it is necessary to add a potential which becomes strongly repulsive when a collective variable corresponding to the distance between two fission fragments becomes large. For the symmetric fission of a four-particle system, a symmetric operator which accomplishes this is

$$U = \sum_{ijk\ell} \theta(x_\ell - x_j)\theta(x_\ell - x_i)\theta(x_k - x_j)\theta(x_k - x_i) U\left[\frac{x_k + x_\ell - x_i - x_j}{2}\right]. \tag{23}$$

In the ordered subspace, U is a function of $R = \frac{x_4 + x_3 - x_2 - x_1}{2}$ which is just the desired separation of the two fragments. Equation (23) may be generalized straightforwardly to larger systems and arbitrary numbers and species of fragments by appropriate groupings of θ-functions.

As in the single-particle case, the energy is easily evaluated by a matrix element of the form in eq.(6). The kinetic energy operator acts upon the trial function eq.(22) and the resulting function is sampled stochastically. Center-of-mass motion may be treated either by working in the cm and evaluating the intrinsic hamiltonian, which requires the calculation of mixed derivatives of the form $\sum_{i\neq j} P_i P_j$ acting on $\hat{\Phi}$, or by adding a one-body harmonic oscillator potential acting on the cm coordinate and explicitly subtracting $\frac{1}{2}\hbar\omega$. When the trace is calculated, the energy is best evaluated using the virial theorem, eq.(12c). It is straightforward to verify for a two-body potential $v(|x_i - x_j|)$ and a potential of the form eq.(23) that the total energy is obtained by replacing v(x) by $\hat{v}(x) = v(x) + \frac{1}{2}xv'(x)$ and U(R) by $\hat{U}(R) \equiv U(R) + \frac{1}{2}RU'(R)$.

C) One-Dimensional Model

In order to construct a one-dimensional model as relevant as possible to nuclear physics, it is desirable to define a saturating system interacting with a two-body potential exhibiting the qualitative behavior of the nuclear force. To define the potential quantitatively, it is useful to require that relevant dimensionless ratios be comparable in one and three dimensions. The fundamental length scale in a saturating system is specified by the saturation density ρ_0, so we define

$$\ell_0 = \rho_0^{-1/D} \tag{24a}$$

where D is the dimension. To within uninteresting geometrical constants, ℓ_0 specifies the characteristic distance between particles. The Schrodinger equation may then be reduced to dimensionless form by measuring all lengths in units of ℓ_0 and energies in units of

$$E_0 = \frac{\hbar^2}{m\ell_0^2} \tag{24b}$$

The potential used in this work is graphed in Figure 1 and was defined such that the scaled binding energy per particle, $\frac{E/A}{E_0}$, fermi gas kinetic energy per particle $\frac{T/A}{E_0}$, core radius $\frac{r_0}{\ell_0}$, and maximum attraction $\frac{V_{max}}{E_0}$ are roughly comparable to the three-dimensional values shown in Table 1. The explicit form of the potential is

$$V(x) = \sum_{i=1}^{2} \frac{V_i}{\sigma_i\sqrt{\pi}} e^{-\frac{x^2}{\sigma_i^2}} \tag{25}$$

with $V_1 = 12$, $V_2 = -12$, $\sigma_1 = 0.2$ and $\sigma_2 = 0.8$ in units such that $\hbar = m = 1$ and $\rho_0 \sim 1.25$.

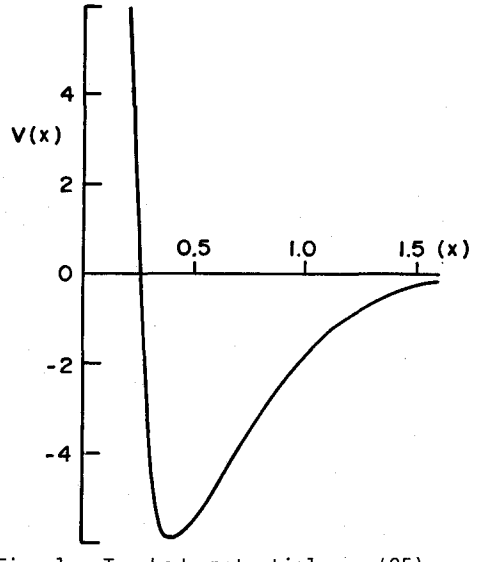

Fig. 1. Two-body potential, eq.(25), used in the one-dimensional model.

Table 1

Comparison of Characteristic Scaled Quantities in Nuclear Matter and the One-Dimensional Model

	D=3	D=1
$\frac{E/A}{E_0}$	-0.09	-0.07
$\frac{T/A}{E_0}$	0.13	0.17
$\frac{r_0}{\ell_0}$	1.25	0.98
$\frac{V_{max}}{E_0}$	0.56	0.39

A crucial consideration in practical calculations is extrapolation of observables as the time step $\varepsilon \to 0$. One can show that the symmetrized expression, eq.(5), used in this work is formally accurate to order ε^2, but one still needs to know how small ε must be in order for quadratic convergence to set in. Heuristically, since the gaussian factor in eq.(5) confines $\Delta x \sim \sqrt{\varepsilon}$ and the smallest characteristic scale of variation of the potential is 0.2, one would expect to see convergence at $\varepsilon \sim (0.2)^2 = 0.04$. Monte Carlo calculations of the binding energy of nuclear matter, obtained by placing 6 particles in a periodic cell, are shown in Figure 2 as a function of ε. One observes that the heuristic estimate $\varepsilon \sim 0.04$ is quite reasonable and that both the normalization energy and trial energy in the initial-value formulation yield consistent and suffici-

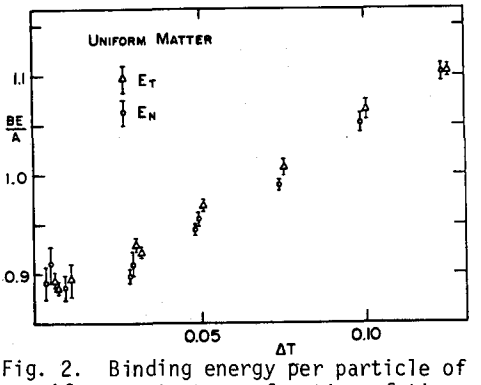

Fig. 2. Binding energy per particle of uniform matter as a function of time mesh size $\varepsilon = \Delta T$. The trial energy, E_T, and normalization energy, E_N, were calculated using 10^4 to 10^5 events.

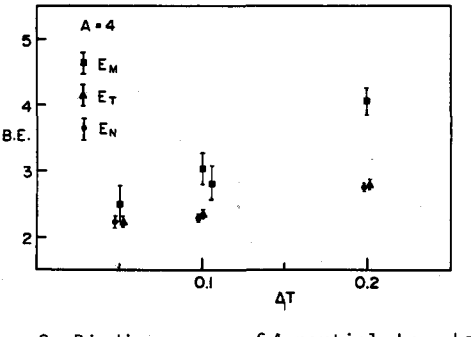

Fig. 3. Binding energy of 4-particle bound state as a function of time mesh size $\varepsilon = \Delta T$ using 10^4 events. The trial energy, E_T, and normalization energy, E_N, were calculated using the initial value form and the energy E_M was obtained using the Metropolis algorithm to evaluate the trace.

ently accurate results with of the order of 10^4 to 10^5 independent events. An analogous calculation of the binding energy of a four-particle bound state is shown in Figure 3 on a compressed scale using roughly 10^4 events. Whereas the variance and convergence with ε of the energies computed from the initial value form are comparable to those in Figure 2, one observes that evaluation of the trace by the Metropolis algorithm using the virial theorem energy expression yields variances roughly four times larger and somewhat less accuracy for large ε. The superior accuracy and variance of the initial value form is obvious from eq.(6). If Φ were the exact ground state, sampling the numerator and denominator with any set of x's would yield the exact energy with zero variance. To the extent to which Φ is a good approximation, it will thus compensate for error in the x's resulting either from statistical fluctuations or from a large value of ε. The importance-sampled version of the trace calculation would presumably yield comparable precision. The nuclear matter saturation curve obtained from a sequence of calculations analogous to that of Figure 2 is shown in Figure 4. In all these calculations, six particles were placed in a cell with periodic boundary conditions and the density was varied by changing the length of the cell. When the cell is made sufficiently large, the six particles form a bound state, so the low density limit is simply a constant equal to the binding energy per particle of a six-particle state. When more particles are included in the cell the surface energy contributes less. Hence, the low-density constant region approaches closer to the saturation point and in the infinite volume limit the saturation curve is constant below the saturation point. Calculated binding energies for 2 to 16 particles are well reproduced by a semi-empirical formula of the form $BE(A) \sim E_0 A - E_s$ where E_0 is the binding energy at saturation, -1.06, and the surface energy E_s is $\sim$1.7.

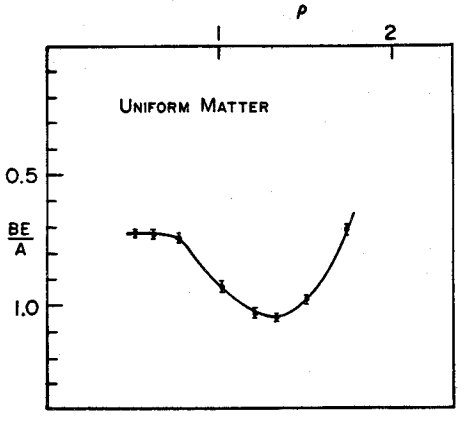

Fig. 4. Saturation curve calculated for six particles in a periodic cell.

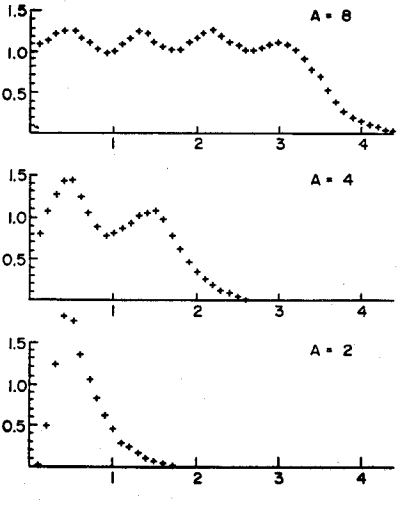

Fig. 5. Ground state density distributions for two, four, and eight-particle bound states.

In order to produce spontaneous fission, a long-range repulsive interaction must be added to the Hamiltonian analogous to the Coulomb interaction. In the present case, the range and strength were adjusted such that a twelve-particle system was stable with respect to single-particle emission and was unstable with respect to fission into two six-particle fragments.

Ground-state density distributions for three nuclei with this force are shown in Figure 5. Note that due to the long-range repulsion, the average interior density is slightly lower than the saturation density $\rho_0 = 1.25$ (defined without this repulsion). The quantum density fluctuations are especially interesting. In the two-body system, antisymmetry forces the density to vanish at the origin, and the size of the low-density region is increased by the repulsive core. In nuclei as large as A=8, the density fluctuations are comparable to those arising in the Hartree-Fock approximation, and a detailed comparison with mean-field theory would be most instructive.

Calculations of barrier penetration are at present still preliminary pending a thorough study of statistical ncertainties. In the case of ground state properties displayed in Figures 2-5, it was extremely valuable to have several independent calculations of the same observable so as to critically assess the accuracy and statistical errors of each separate calculation. The primary problem in the tunneling calculation is the fact that two grossly different energy scales entering into the problem simultaneously place very stringent demands on the calculation. On the one hand, as seen already in Figure 2, the strong repulsive core requires that the time step ε be very small. On the other hand, the collective motion through the barrier involves a large mass moving in a large double well potential so that calculation of the energy splitting requires the total time, $\beta=N\varepsilon$, to be large. Hence, N must be very large, on the order of 10^4 or 10^5. The fundamental problem with such a large time lattice is assuring that true equilibrium has been reached which is genuinely independent of the initial condition. The ultimate physics objective, of course, is to understand just this interplay between two-body correlations involving the large energy scale and the collective dynamics involving the low energy scale, and it is not surprising that this complicated physics question should ultimately translate into a correspondingly complicated stochastic calculation.

Straightforward modifications may be introduced into both the initial-value and trace calculations described above to improve the statistics relevant to the collective dynamics. In both cases, the key is to explicitly introduce the collective variable discussed in connection with eq.(23), which for symmetric fission is $R = \frac{2}{N}[\sum_{i=N/2+1}^{N} x_i - \sum_{i=1}^{N/2} x_i]$. In the initial-value form, it is convenient to introduce importance sampling into the numerator of the many-body generalization of eq.(10) using a function $\phi \sim e^{-\alpha R}$. This function generates a net drift of the collective motion from the right well to the left, thereby significantly improving the statistics.

In using the Metropolis algorithm to evaluate the trace, a convenient means of facilitating equilibration of the collective variable is to explicitly vary the variable R at each time step, as well as each of the individual coordinates x_i. As remarked in the

discussion of the Metropolis algorithm, any change in the configuration accepted or rejected on the basis of the change in the action satisfies the reversibility condition, eq.(16), and thus yields the correct equilibrium distribution. Whereas it would take many individual random changes of each coordinate to move two fragments a significant distance from each other, it is clear that a much smaller number of random steps in R will fully explore this degree of freedom. Preliminary results to date show the expected qualitative behavior in the evolution of R. As in the case of a single particle in a double well, the trajectory of R is comprised of regions of fluctuations around the parent ground state and the two fragment scission point, connected by instanton-like paths through the fission barrier. It now remains to obtain a statistically reliable correlation function, eq.(14), from which the energy splitting may be determined, and to confirm the result with the corresponding initial-value evaluation using eq.(10).

D) Future Prospects

On the basis of these initial calculations, it is clear that the model problem described above can be solved to the required accuracy and compared in detail with mean field theory. Comparison of exact ground states with various mean field calculations is already a rich testing ground for approximations presently utilized in nuclear theory. One can define classes of Skyrme forces to reproduce the exact mass table and saturation density and then directly compare a number of observables. This should give significant insight, for example, into the role of the effective mass and compression modulus. More microscopic approximations, such as the Brueckner G-matrix, systematic truncation of the coupled-cluster hierarchy, RPA corrections, etc. may also be definitively explored. Given an acceptable ground state approximation, one may then compare the SPA result using the bounce equations eq.(18) with an exact solution to explore the validity of the SPA and the use of a ground state effective interaction. One may thus expect to obtain insight into a variety of approximations which are presently used but not understood.

Physics in three dimensions, of course, is much different and richer than in one dimension. It is well-known, for example, that one-dimensional systems don't undergo phase transitions, that mean field theory breaks down near the critical point, and that two-body collisions cannot yield dissipation. Given the scale of the computational problem in one dimension, however, it is not likely that treatment of realistic potentials in higher dimensions will be practical in the near future. Exact solutions to interesting problems do not come easily, so at this stage all I can suggest is to be patient, to think hard about the physics contained in the one-dimensional problem which is presently accessible to us, and to savor the insight thus obtained.

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