Quasiparticle model for nuclear dynamics studies: Ground-state properties

David H. Boal and James N. Glosli
Department of Physics, Simon Fraser University, Burnaby, British Columbia, Canada V5A 1S6
and TRIUMF, Vancouver, British Columbia V6T 2A3
(Received 16 February 1988)

A model Hamiltonian is advanced which provides a computationally efficient means of investigating nuclear dynamics. The Hamiltonian includes both Coulomb and isospin-dependent terms, and incorporates antisymmetrization effects through a momentum-dependent potential. Unlike many other classical or semiclassical models, the nuclei of this simulation have a well-defined ground state with a nonvanishing $\langle p^2 \rangle$. It is shown that the binding energies per nucleon and rms radii of these ground states are close to the measured values over a wide mass range.

I. INTRODUCTION

This paper is the first in a sequence of three which will develop a model which is both computationally fast and describes many of the properties of nuclei and their reactions at energies of less than 200 A MeV. In this paper, the main ingredients of the model will be outlined, and its ground-state properties will be explored. In the second paper, the problems of handling collisions in a stochastic manner which preserves angular momentum will be dealt with. The last paper in the series will deal with the thermodynamic properties of the model, particularly its phase structure.

Finding a model description of nuclei which can be handled in an efficient manner for computer simulations is a difficult task. On a quantum mechanical level, the wave functions must be antisymmetrized because of the fermionic nature of the nuclear constituents, and this implies that one is dealing with $N!$ components to the wave function even for a single Slater determinant. It is clear that determining the time evolution of anything but the lightest nuclei by numerically propagating the nuclear wave function would be computationally very demanding. Many of the computational models which have been advanced, particularly for the study of nuclear fragmentation which involves evaluating many-body correlations, attempt to reduce the N-body problem to one which involves the evaluation of only N^2 elements for a force or energy. While it is recognized that such simplifications may not always be particularly accurate, such N^2 models, as we will call them, appear to be the only ones fast enough to be reliably evaluable in a typical Monte Carlo calculation. In other words, one is forced to make a compromise between approximating the many-body physics and producing a simulation which can execute fast enough to produce a statistically significant Monte Carlo sample. The sample size may run from a few hundred events to calculate a mass yield curve from a reaction, up to tens of thousands of events to predict a correlation function.

The difficulty in performing the N^2 reductions lies less in the nuclear potential (models of which are often obtained from the analysis of nucleon-nucleon scattering—a two-body process) than in the problem of enforcing the necessary restrictions on the occupancy of states required by Fermi-Dirac statistics. For the time evolution of one-body distributions, incorporating the effects of the Pauli principle are not overly difficult. Once one has an initial state which satisfies the constraints on phase-space occupancy (this is not a totally trivial task) then the distribution can be propagated by means of a collisionless transport equation without violating the phase-space constraints. Introducing a collision term for fermions, as suggested by Nordheim[1] and Uehling and Uhlenbeck[2] (which we will call the NUU method) may cause problems for the computer simulation of many-body distributions.

The essence of the NUU method is the following: Each time a collision occurs, a tentative assignment is made for the new momenta of the scattered pair of particles according to a predetermined distribution. The occupancy of the tentative phase space determines whether the collision is allowed. In a Monte Carlo simulation, the determination of whether a collision is allowed is made by comparing a random number with the occupancy. This method has been applied to simulations of the time evolution of one-body and A-body distributions.[3–7]

To see how the NUU collision term will affect the time evolution of many-body distributions, let us focus on the initialization problem. That part of the energy density associated with the nuclear force is often parametrized in the simple form:

$$H(r)=\frac{A}{2}\frac{\rho(r)^2}{\rho_0}+\frac{B}{3}\frac{\rho(r)^3}{\rho_0^2} \ . \tag{1}$$

Here A and B are constants, ρ_0 is the density of normal nuclear matter taken to be 0.17 fm^{-3}, and isospin and other terms have been neglected. For infinite uniform nuclear matter, the energy per nucleon corresponding to Eq. (1) has a minimum value of -41.22 MeV at $\rho=1.33\rho_0$. A finite system of classical computational nucleons will thus have a ground-state energy in this range as well.

This classical computational ground state is, of course, not what one wants for nuclei. One method used to help

avoid this problem is simply to start with a phase-space distribution which is closer to what is expected of the "real" nucleus and propagate it. In a Monte Carlo approach, this distribution will have fluctuations, the magnitude of which depend on the individual model. If the fluctuations in the initialization are large, then the NUU collision term will help smooth them out by scattering particles away from high-density regions to low-density ones. On the other hand, if considerable care has been taken to initialize the phase space (such as is done in Ref. 4 for one-body distributions) then the collision term may actually induce unwanted fluctuations in the many-body distributions of cold nuclei. This can happen when an unlikely collision occurs and transfers a particle into a region of phase space which is already nearly saturated, thus oversaturating the region. These phase-space fluctuations generally cause the computational nuclei to be metastable, although the lifetimes may be very long.

In models such as Refs. 5–7, the indeterminacy of the binding energies of these metastable states is typically 1–2 MeV per nucleon. This puts a fundamental uncertainty on the excitation of these nuclei which is not present in, for example, molecular dynamics calculations. Hence, when one of these models[8,9] was used to investigate the effects of the liquid-vapor phase transition on nuclear reactions, only the reaction trajectories in phase space could be evaluated, not trajectories in the excitation energy versus density plane.[10] The need for a well-defined ground state is even more obvious when one wishes to make comparisons with data, particularly mass distributions. The simulation must be capable of calculating excitation energies and, equally important, must possess a prescription for following the decays of these excited states.[11]

An alternative to the NUU method is to add to the nuclear and Coulomb terms a classical potential whose ground state for noninteracting particles resembles a Fermi gas. Parametrized functional forms for such potentials have been advanced by several groups,[12–14] beginning a decade ago. What we wish to do here is obtain a potential from the expectation value of the kinetic-energy operator for a specific nuclear wave function, so that a physical meaning can be attached to the parameters of the potential. The functional form we obtain bears some resemblance to at least one of the previous ansatze.[13]

The layout of the paper is as follows. In Sec. II we derive what we call the Pauli potential, and investigate its ground-state properties. Of course, to have a model relevant to nuclei, we need a strong interaction Hamiltonian, and this is obtained in Sec. III. Finally, the ground states of finite nuclei governed by the combined nuclear and Pauli Hamiltonian are summarized in Sec. IV.

II. A PAULI POTENTIAL

One of the most important effects of Fermi-Dirac statistics as far as a nucleus is concerned is that the ground state is forced to have a nonzero expectation value of the kinetic-energy operator:

$$\langle K \rangle = -\frac{\hbar^2}{2m}\left\langle \Psi_{\text{g.s.}} \left| \sum_i \nabla_i^2 \right| \Psi_{\text{g.s.}} \right\rangle , \tag{2}$$

where all nucleons will be assigned a mass m of 938.9 MeV in this calculation. We wish to express Eq. (2) in terms of a set of quasiparticles. The antisymmetrization of the wave function causes the evaluation of Eq. (2) to include a summation over at least $N!$ terms and possibly as many as $N(N!)^2$ terms. This is computationally prohibitive for all but the very lightest systems. To consider nuclei of the order of 10^2 nucleons, one is restricted to calculations of order N^2 in complexity. Hence we seek approximations which allow us to express Eq. (2) in terms of two-body interactions between the quasiparticles.

Consider the two-particle problem. We take the single-particle wave functions, before antisymmetrizing, to be Gaussian wave packets

$$\chi_a(\mathbf{r}) = \left[\frac{\alpha^2}{\pi}\right]^{3/4} \exp\left[-\frac{\alpha^2(\mathbf{r}-\mathbf{r}_a)^2}{2}\right] \exp\frac{i\mathbf{p}_a\cdot\mathbf{r}}{\hbar} \tag{3}$$

centered at $\mathbf{r}_a$ with average momentum $\mathbf{p}_a$. The width of the wave packet is characterized by the parameter α. The two-particle wave function is then

$$\Psi_{ab}(\mathbf{r}_1,\mathbf{r}_2) = \frac{\chi_a(\mathbf{r}_1)\chi_b(\mathbf{r}_2)-\chi_a(\mathbf{r}_2)\chi_b(\mathbf{r}_1)}{\left[\int\int |\chi_a(\mathbf{r}_1)\chi_b(\mathbf{r}_2)-\chi_a(\mathbf{r}_2)\chi_b(\mathbf{r}_1)|^2 d\mathbf{r}_1 d\mathbf{r}_2\right]^{1/2}} . \tag{4}$$

The total kinetic energy of the particle pair can be shown to be

$$\langle K \rangle_{ab} = \frac{1}{2m}\left[\mathbf{p}_a^2+\mathbf{p}_b^2+3\alpha^2\hbar^2+\alpha^2\hbar^2\frac{X_{ab}}{e^{X_{ab}}-1}\right] , \tag{5}$$

where

$$X_{ab} = \tfrac{1}{2}[\alpha^2(\mathbf{r}_a-\mathbf{r}_b)^2+(\mathbf{p}_a-\mathbf{p}_b)^2/(\hbar^2\alpha^2)] .$$

The $3\alpha^2\hbar^2$ term reflects the fact that the wave packet is not a delta function in momentum.

From the form of Eq. (5), we can identify the last term as a two-body potential between quasiparticles with phase-space coordinates $(\mathbf{r}_a,\mathbf{p}_a)$ and $(\mathbf{r}_b,\mathbf{p}_b)$:

$$V_p(X_{ab}) = \frac{\alpha^2\hbar^2}{2m}\frac{X_{ab}}{e^{X_{ab}}-1} , \tag{6}$$

which will be referred to as the Pauli potential. The potential has the following desirable properties: In the limit in which the quasiparticles are well separated in phase space, i.e., $X_{ab}\to\infty$, the potential vanishes. Further, the potential is repulsive for finite separations in phase space. Qualitatively, this is the behavior which we expect for the

many-particle Fermi gas.

It remains to be demonstrated that the ground state of an N-body system of quasiparticles interacting via Eq. (6) resembles that of an ideal Fermi gas. With our model, the energy of the N-particle Fermi gas would be

$$E(\mathbf{r},\mathbf{k})=\frac{\hbar^2\alpha^2}{2m}\left[\sum_l (k_l/\alpha)^2+\tfrac{1}{2}\sum_{l\neq m}\frac{X_{lm}}{e^{X_{lm}}-1}\right], \quad (7)$$

where

$$X_{lm}=\tfrac{1}{2}(\alpha^2 r_{lm}^2+k_{lm}^2/\alpha^2),$$

$$\mathbf{k}_l=(k_l^x,k_l^y,k_l^z), \quad \mathbf{r}_l=(r_l^x,r_l^y,r_l^z),$$

$$\mathbf{k}_{lm}=\mathbf{k}_l-\mathbf{k}_m, \quad \mathbf{r}_{lm}=\mathbf{r}_l-\mathbf{r}_m,$$

and where $\hbar\mathbf{k}_a=\mathbf{p}_a$.

As an example of what happens in a many-body system, consider the particles placed on a cubic lattice with lattice spacing a. If $a\alpha\gg 1$, then the sites are effectively decoupled, and the ground state has $\mathbf{k}_l=0$ for all l. For small $a\alpha$ this is not the case. We will show that as $a\alpha$ is reduced the $\mathbf{k}_l=0$ configuration changes from a local minimum of the energy to a saddle point. We begin by considering the nature of E as a function of $\mathbf{k}_l$ near the point $\mathbf{k}_l=0$. First note that $\partial E/\partial k_l^\mu=0$ for all l and $\mu=x,y,z$. Hence $\mathbf{k}_l=0$ is a critical point of E. Now consider the curvature matrix of E at $\mathbf{k}_l=0$

$$M_{l\mu;m\nu}=\left.\frac{\partial^2 E}{\partial k_l^\mu \partial k_m^\nu}\right|_{k=0}$$

$$=\frac{\hbar^2}{m}\delta_{\mu\nu}\begin{cases}1+\sum_{j\neq l} f(\frac{1}{2}\alpha^2 r_{lj}^2), & l=m,\\ -f(\frac{1}{2}\alpha^2 r_{lm}^2), & l\neq m,\end{cases} \quad (8)$$

where

$$f(X)=\frac{1}{e^X-1}-\frac{Xe^X}{(e^X-1)}.$$

In the limit $N\to\infty$, all lattice sites are equivalent, and the sum over particle label can be replaced by a sum over lattice sites:

$$\sum_{j\neq l} f(\tfrac{1}{2}\alpha^2 r_{lj}^2)=\sum_{\substack{r\neq 0\\ r\in\text{lattice}}} f(\tfrac{1}{2}\alpha^2 r^2).$$

Defining

$$Q(X^2)=\begin{cases}1+\sum_{\substack{r\neq 0\\ r\in\text{lattice}}} f(\frac{1}{2}\alpha^2 r^2), & X=0,\\ -f(\frac{1}{2}X^2), & X\neq 0,\end{cases} \quad (9)$$

then Eq. (8) can be rewritten

$$M_{l\mu;m\nu}=\frac{\hbar^2}{m}\delta_{\mu\nu}Q(|\mathbf{r}_l-\mathbf{r}_m|^2).$$

It will be demonstrated that

$$[\mathbf{V}(q)]_{m\nu}=e^{-i\mathbf{r}_m\cdot\mathbf{q}}\omega_\nu$$

is an eigenvector of M for all $\mathbf{q}=(q^x,q^y,q^z)$, $q^\mu\in(-\pi/a,\pi/a)$,

$$M\mathbf{V}(\mathbf{q})=\sum_{m\nu} M_{l\mu;m\nu}e^{-i\mathbf{r}_m\cdot\mathbf{q}}\omega_\nu$$

$$=\frac{\hbar^2}{m}\sum_{m\nu}\delta_{\mu\nu}Q(|\mathbf{r}_l-\mathbf{r}_m|^2)e^{-i\mathbf{r}_m\cdot\mathbf{q}}\omega_\nu$$

$$=\frac{\hbar^2}{m}\sum_{m\nu}\delta_{\mu\nu}\omega_\nu(Q|\mathbf{r}_l-\mathbf{r}_m|^2)\times e^{i(\mathbf{r}_l-\mathbf{r}_m)\cdot\mathbf{q}}e^{-i\mathbf{r}_l\cdot\mathbf{q}}. \quad (10)$$

Replacing the sum over particle label by the sum over lattice sites,

$$M\mathbf{V}(\mathbf{q})=\frac{\hbar^2}{m}\omega_\mu e^{-i\mathbf{r}_l\cdot\mathbf{q}}\sum_{r\in\text{lattice}} Q(|r|^2)e^{-i\mathbf{r}\cdot\mathbf{q}}$$

$$=\lambda(\mathbf{q})\mathbf{V}(\mathbf{q}) \quad (11)$$

where

$$\lambda(\mathbf{q})=\frac{\hbar^2}{m}\sum_{r\in\text{lattice}} Q(|r|^2)e^{-i\mathbf{r}\cdot\mathbf{q}}$$

$$=\frac{\hbar^2}{m}\left[1+\sum_{r\in\text{lattice}} f(\tfrac{1}{2}\alpha^2 r^2)[1-\cos(\mathbf{r}\cdot\mathbf{q})]\right].$$

So $\mathbf{V}(\mathbf{q})$ is an eigenvector of M with eigenvalue $\lambda(\mathbf{q})$. The minimum of $\lambda(\mathbf{q})$ occurs along the line $q^x=q^y=q^z$ for all α. From Fig. 1 we see that for $a\alpha>2.2$, $\lambda(\mathbf{q})>0$ for all $\mathbf{q}$ hence $\mathbf{k}_l=0$ is a local minimum (in fact the global minimum). If $a\alpha<2.2$., $\lambda\mathbf{q}$ will change sign as a function of $\mathbf{q}$ which implies that $\mathbf{k}_l=0$ is a saddle point and cannot be the global minimum of E. So the ground state of

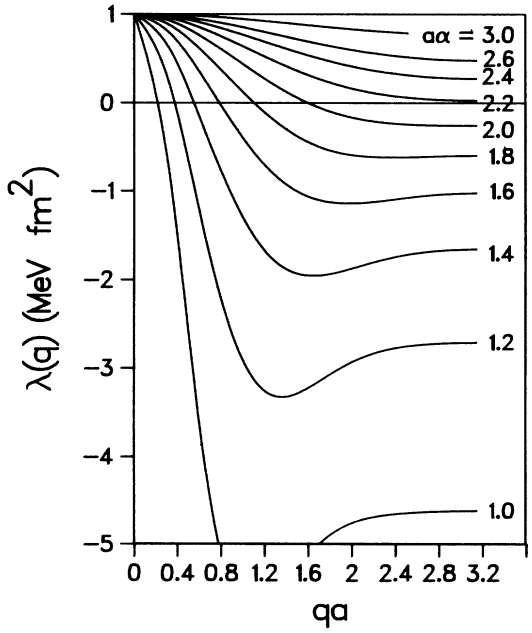

FIG. 1. Eigenvalues of the curvatures matrix along $q_x=q_y=q_z$ axis for various values of $a\alpha$.

the system will exist for some nonzero value of $\mathbf{k}_l$. For example, for $a\alpha$ slightly less than 2.2, the ground state is one in which $\mathbf{k}_l$ alternates in sign with lattice position corresponding to $qa=\pi$. As $a\alpha$ is decreased further, the direction of greatest negative curvature at the $\mathbf{k}_l=0$ state shifts to lower values of qa. For example, qa is significantly less than $\pi/2$ at $a\alpha=1.0$. One expects the minimum in the energy will also shift in this direction.

Having demonstrated that the ground state of a system of these quasiparticles can possess a nonzero kinetic energy, it remains to be shown that the energy of this system can be brought into quantitative agreement with that of a Fermi gas. The energy of the quasiparticle ground state depends upon α, which up until this point has been treated as a free parameter. We wish to fix α by demanding that the ground-state energy of the system of quasiparticles on a simple cubic lattice be close to that of an ideal Fermi gas at the equivalent density. However, we find that Eq. (6) as it is written will always underestimate the energy of a Fermi gas over all ranges of α.

The reason for this lies in the fact that we retained only two-body terms in evaluating the kinetic energy of the many-body system. To estimate the magnitude of this approximation, consider the simple one-dimensional system three particles equally spaced on a straight line. Using the single-particle wave functions of Eq. (3), one can calculate the exact kinetic energy of the fully antisymmetrized three-body wave function via

$$\langle K\rangle_3=\frac{\int\int\int \Psi^*_{abc}(x_1,x_2,x_3)(\hat{K}_1+\hat{K}_2+\hat{K}_3)\Psi_{abc}(x_1,x_2,x_3)dx_1\,dx_2\,dx_3}{\int\int\int \Psi_{abc}(x_1,x_2,x_3)\Psi_{abc}(x_1,x_2,x_3)dx_1dx_2dx_3}\ . \tag{12}$$

The antisymmetrized wave function $\Psi_{abc}(x_1,x_2,x_3)$ is formed via

$$\Psi_{abc}(x_1,x_2,x_3)=\frac{1}{\sqrt{3!}}\sum_{ijk}\epsilon_{ijk}\chi_a(x_i)\chi_b(x_j)\chi_c(x_k)\ ,$$

where ϵ_{ijk} is the totally antisymmetric Levi-Civita tensor. The kinetic energy in Eq. (12) is to be compared with the pairwise result of

$$\langle K\rangle_{\text{pair}}=\tfrac{1}{2}\sum_{i\neq j}\langle K\rangle_{ij}$$

with $\langle K\rangle_{ij}$ defined by Eq. (5). The ratio $R=\langle K\rangle_3/\langle K\rangle_{\text{pair}}$ is dependent on the relative positions of the particles in phase space: The further the particles are separated, the closer R will be to unity. Taking $k_a=k_b=k_c=0$ to obtain an upper bound, we find R will range up to about 1.5 depending on αa. This is an upper limit for R, in that all momenta have been set equal to zero even though αa is in a range where this momentum configuration is not the ground state. For the true one-dimensional ground state, the three-body terms will not be as large. However, in moving from the three-body system in one dimension just considered to the many-body system in three dimensions, we expect that the many-body terms will be the same order of magnitude as the pair terms.

Hence, we are forced to rescale the strength of the Pauli potential, which we write as:

$$V_p(X_{ab})=V_s\frac{\alpha^2\hbar^2}{2m}\frac{X_{ab}}{e^{X_{ab}}-1}\ . \tag{13}$$

This rescaling, which is required to reproduce the energetics of the three- and higher-body systems, means that the energy of the isolated two-body system is overpredicted. However, it is far more important to have the many-body energy correct. As we discuss below, the characteristics chosen for nuclear interaction will also be weighted towards the heavier systems, although the model does handle light systems reasonably well.

The two parameters of the potential, V_s and α, are estimated by equating the ground-state energy per particle of a simple cubic lattice at a specific density with that of an ideal Fermi gas at the same density. Three densities are chosen for comparison, $\rho_s/2$, ρ_s, and $2\rho_s$, and for each a locus of values of V_s and α which yield the same energy as the Fermi gas are obtained. The reference density ρ_s is equal to $\rho_0/4$ to take into account the four spin degrees of freedom in nuclei. The specific lattice chosen had 4^3 sites with periodic boundary conditions imposed by working on an 8^3 (i.e., two periodic sites along each side) lattice. It was found that making the lattice larger (6^3 with two periodic sites along each side) did not change the energy appreciably. The ground state was determined by a Monte Carlo algorithm in which random changes are made to the momenta of pairs of particles, and the changes are accepted or rejected according to whether they lower the energy of the system. Lastly, it should be noted that the energy of the lattice at infinite lattice spacing is finite (the energy per particle is $3\alpha^2\hbar^2/2m$). In order to compare with the ideal Fermi gas result, whose energy vanishes at zero density, the energy of the lattice at infinite separation has been subtracted from that at finite separation.

The results are shown on Fig. 2 for the three densities. One can see that there is a common intersection area around $V_s=1.7-1.9$ and $\alpha=\frac{1}{2}$ fm^{-1}. This value for V_s is just what we expect from the discussion above on many-body corrections. Further, the value of α can be compared with results obtained in our previous semiclassical equations of motion (SCEOM) model.[8,9] In that model, the Wigner transform of the wave functions in Eq. (3) was used to construct a classical phase space for fermions. It was found that in order to minimize the fluctuations in that phase space for "cold" nuclear matter, α had a value of $\frac{1}{2}$ fm^{-1}, identical to the result here.

Having examined the accuracy with which our Pauli potential reproduced the ground-state energy of an infinite system of fermions, we now apply it to a finite system of particles in an external potential. The specific case

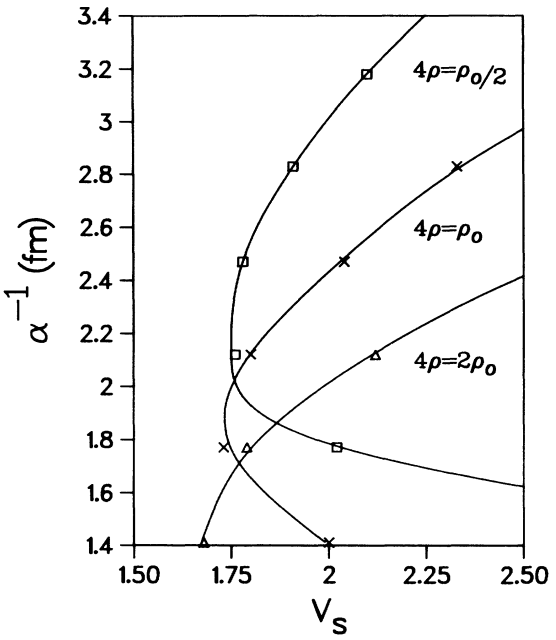

FIG. 2. Loci of values of V_s and α^{-1} which produce the same ground-state energy for the simple cubic lattice as the ideal Fermi gas. The loci are shown for three densities: $\rho_s/2$, ρ_s, and $2\rho_s$, where $\rho_s=\rho_0/4$.

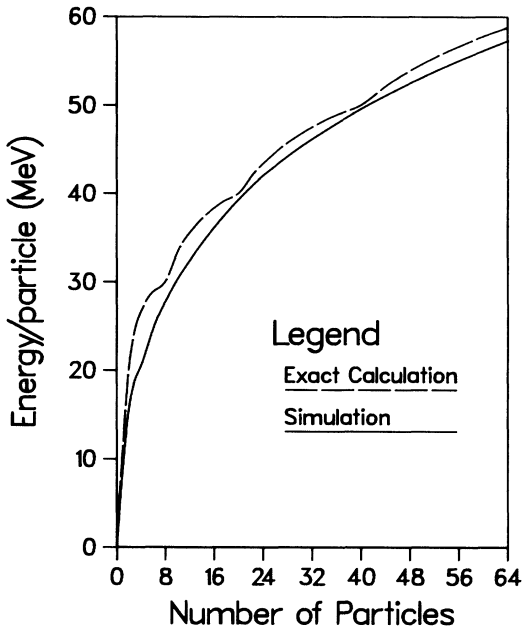

FIG. 3. Ground-state energy per particle calculated for a system of noninteracting neutrons in a harmonic potential with $k=4.038$ MeV/fm^2. The dashed curve refers to the exact quantum mechanical calculation, while the solid curve is the result from the simulation.

we examine is that of a harmonic potential, because of the availability of an exact quantum mechanical solution. The system consists of an equal number of spin-up and spin-down neutrons (with no nuclear interaction) subject to a harmonic potential of the usual form $\frac{1}{2}kx^2$. A harmonic oscillator fit to the ground-state properties of ^{16}O gave[15] $k=4.038$ MeV/fm^2, which we will use as a representative value for finite nuclear systems. For $\alpha=\frac{1}{2}$ fm^{-1}, we do not find a large change in our predictions of the ground-state energy as V_s is varied from 1.7 to 1.9, although 1.9 is in somewhat better agreement with the exact result. Both the exact calculation and the results from the simulation are shown in Fig. 3. The agreement between the two calculations is good, although of course we cannot reproduce the structure associated with shell closings. From this calculation and the infinite lattice results, we fix $\alpha=\frac{1}{2}$ fm^{-1} and $V_s=1.9$.

Finally, it is worthwhile commenting on the relationship between this potential and the ansatze advanced previously. We have not attempted a comparison between the ground-state properties of our potential and that of Refs. 12 and 13; we have not solved for the ground states associated with our nuclear interaction and either alternate Pauli potential nor do we claim that ours produces a more realistic ground state. The strength of this approach is that the potential is derivable under a set of approximations, and the two parameters can then be estimated by independent methods. It is encouraging that the values of the parameters obtained in the fit to the Fermi energy are consistent with these general expectations. It is also encouraging to note that the functional form which we obtain for the potentials is not too dissimilar to those used previously, particularly Ref. 13.

III. NUCLEAR INTERACTION

A. The quasiparticle potential

The functional form we choose for the nuclear potential energy density is derivable from a zero-energy Skyrme interaction[16]

$$V=\frac{A}{2}\frac{\rho^2}{\rho_0}+\frac{B}{3}\frac{\rho^3}{\rho_0^2}+\frac{C}{2}\frac{(\rho_p-\rho_n)^2}{\rho_0}+\frac{g_1}{2}(\nabla\rho)^2 . \tag{14}$$

These first two terms are the same as those in Eq. (1). The third term is isospin dependent and is a function of the proton and neutron densities, ρ_p and ρ_n, respectively. The fourth term depends on the gradient of the density and can also be motivated by the Skyrme interaction. We discuss the determination of the parameters A, B, C, and g_1 below.

To evaluate the total energy, we assume that the partial density ρ can be written as

$$\rho(r)=\sum_i \rho_i(r) ,$$

where the sum runs over all particles i. This assumption is equivalent to saying that the cross terms in the $\Psi^*\Psi$ product of antisymmetrized single-particle wave functions cancel. Taking the wave packets of Eq. (4), $\rho(r)$ becomes

$$\rho(\mathbf{r})=\left[\frac{\alpha}{\sqrt{\pi}}\right]^3\sum_i \exp[-\alpha^2(\mathbf{r}-\mathbf{r}_i)^2] . \tag{15}$$

We rewrite the expression for the total nuclear potential energy using the shorthand

$$\langle A \rangle_i = \int \rho_i(r) A \, d^3r \ ,$$

from where,

$$\int V \, d^3r = \frac{A}{2} \sum_i \left\langle \frac{\rho}{\rho_0} \right\rangle_i + \frac{B}{3} \sum_i \left\langle \frac{\rho^2}{\rho_0^2} \right\rangle_i + \frac{C}{2} \int \frac{(\rho_p - \rho_n)^2}{\rho_0} d^3r + \frac{g_1}{2} \int (\nabla \rho)^2 \, d^3r \ . \tag{16}$$

Because of the Gaussian form of the density in Eq. (15), all of the integrals in Eq. (16) can be done analytically. Furthermore, all but one of the sums involves only N^2 terms. The problem summation is that over $\langle \rho^2/\rho_0^2 \rangle_i$, which is of order N^3. For a system of hundreds of particles, evaluation of N^3 elements is computationally prohibitive, and so we approximate it by

$$\sum_i \left\langle \frac{\rho^2}{\rho_0^2} \right\rangle_i = \sum_i \left\langle \frac{\rho}{\rho_0} \right\rangle_i^2 + \frac{g_2}{2} \int (\nabla \rho)^2 \, d^3r \tag{17}$$

which is an N^2 operation. For uniform matter, this approximation is of no consequence. However, omission of the second term allows for certain fluctuations which preserve average density to develop with no penalty in energy, and these fluctuations can lead to ground-state instabilities in nuclei past the maximum in the binding energy per nucleon curve. Since g_1 and g_2 multiply the same functional form, they will be subsumed into $G = g_1 + g_2$.

Lastly, the Coulomb potential between protons is included as well. The functional form of the Coulomb potential between two protons with Gaussian charge distributions [i.e., Eq. (4)] contains error functions, which are cpu time consuming to evaluate. Since this is not a critical part of the calculation, we replace the Gaussian density distribution with a uniform spherical distribution. A radius for the sphere of $r_0 = 3\sqrt{2\pi}/4\alpha$ has been chosen to give a potential which approximates the exact potential.

By substituting Eqs. (15) and (17) into Eq. (16) and performing the integrals an explicit form for the interaction between the quasiparticles due to the nuclear potential is found. Combining this with the Pauli and Coulomb potential the energy of a collection of quasiparticles can be written as

$$H = \frac{1}{2M} \sum_i p_i^2 + \tfrac{1}{2} \sum_{i \neq j} [V_p(X_{ij}) + V_c(r_{ij})] + \tfrac{1}{2} \sum_{ij} \left[\frac{(A + C S_i S_j)}{\rho_0} + \alpha^2 G (3 - \alpha^2 r_{ij}^2) \right] D(r_{ij}) + \frac{B}{3\rho_0^2} \sum_i \left[\sum_j D(r_{ij}) \right]^2 , \tag{18}$$

where

$r_{ij} = | \mathbf{r}_i - \mathbf{r}_j |$,

$S_i = 1(-1)$ for protons (neutrons)

and

$$V_c(r) = \frac{e^2}{4\pi\epsilon_0} \begin{cases} 1/r, & r > r_0 \ , \\ [3 - (r/r_0)^2]/(2r_0) & \text{otherwise} \ , \end{cases}$$

$$D(r) = \left[\frac{\alpha}{\sqrt{2\pi}} \right]^3 e^{-\alpha^2 r^2/2} \ .$$

We emphasize that Eq. (18) is an explicit expression for the Hamiltonian in terms of the phase-space coordinates of the quasiparticles. All of the integrals over the probability distributions of the nucleons have been done analytically so that test-particle methods, etc., are not needed. The Hamiltonian then explicitly involves only two-body terms.

B. Parameter determination

The model has a total of six parameters: α and V_s from the Pauli potential as well as A, B, C, and G from the nuclear interaction. The Pauli parameters were determined by approximating the properties of the zero-temperature Fermi gas in the previous section. Once the nuclear parameters have been fixed, then the ground-state properties of any nucleus can be calculated. One method of determining the four nuclear parameters, then, is to calculate the binding energies and rms radii of as many nuclei as is practical and perform a least-squares fit to the experimentally observed values. This approach is exceedingly cpu time consuming within this model.

The approach adopted here is to find constraints imposed by the infinite-nuclear-matter limit so as to reduce the fit to a search over one free parameter. The constraints are as follows.

(i) The binding energy per nucleon of infinite nuclear matter at $\rho = \rho_0 = 0.17$ fm^{-3} and small $\omega = (\rho_p - \rho_n)/\rho_0$ is taken to be[17] $B = E_0 + a_s \omega^2$, where $E_0 = 15.68$ MeV, and $a_s = -28.06$ MeV. (ii) The binding energy has a maximum at $\rho = \rho_0$ and $\omega = 0$.

We can calculate the energy in the infinite-matter limit using Eq. (14) for the potential energy and the ideal Fermi gas result for the kinetic energy. For small ω, the result is

$$E(\rho) = \tfrac{3}{5}\epsilon_F(\rho/\rho_0)^{2/3} + \tfrac{1}{3}\epsilon_F(\rho/\rho_0)^{2/3}\omega^2 + A/2(\rho/\rho_0) + B/3(\rho/\rho_0)^2 + C/2(\rho/\rho_0)\omega^2 \ , \tag{19}$$

where ϵ_F is the Fermi energy at $\rho = \rho_0$ and has the value 38.37 MeV. The binding energy is the difference between Eq. (19) and the energy (E_∞) when the particles are infinitely separated. Typically it is assumed that $\rho \equiv 0$ for infinite separation, therefore $E_\infty = 0$ in Eq. (19). Under this assumption we can solve for A, B, and C to find the respective values -124.11, 70.06, and 30.54 MeV. However, with this model and with real systems the density at infinite separation is not identically equal to zero. The finite wave-packet width of Eq. (4) gives rise to a nonzero E_∞ given by

$$E_\infty = \frac{A}{2}(\rho_1/\rho_0) + \frac{B}{3}(\rho_1/\rho_0)^2 + \frac{C}{2}(\rho_1/\rho_0) + \tfrac{3}{2}G\alpha^2(\rho_1/\rho_0) , \tag{20}$$

where

$$\rho_1 = (\alpha/\sqrt{2\pi})^3 = 0.00794 \text{ fm}^{-3} \text{ at } \alpha = \tfrac{1}{2} \text{ fm}^{-1} .$$

With these three constraints, a one-parameter fit can be performed to the binding energies and rms radii using G as the single parameter. Based on a similar, but different, search performed previously[18] we would expect G to be in the several hundred MeV-fm^5 range. The results are summarized in the next section.

IV. GROUND-STATE PROPERTIES

The calculational method used to find the ground states of a given system is the following: First, an initial choice is made for the positions and momenta of all A nucleons. The initialization is very similar to that used in the SCEOM model:[8,9] Nucleons are placed on a bcc lattice and are then assigned momenta distributed randomly with a sphere in momentum space of radius equal to the local Fermi momentum.

These positions and momenta are allowed to evolve in time according to a set of damped equations of motion:

$$\dot{q}_i = \frac{\partial H}{\partial p_i} - \mu \frac{\partial H}{\partial q_i} , \tag{21a}$$

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} - \frac{\mu}{b}\frac{\partial H}{\partial p_i} , \tag{21b}$$

where μ is chosen to have a value of 400 (fm c/MeV) and b is 938.9 (fm c/MeV)^2. In the $b \to \infty$ limit this technique reduces to that of Ref. 12.

The equations of motion are then integrated using a Runge-Kutta procedure[19] until $\dot{p}_i$ and $\dot{q}_i$ become sufficiently small. Typical values are found to be less than $\dot{q}_i \sim 10^{-2}c$ and $\dot{p}_i \sim \frac{1}{2}$ MeV/fm after 200 fm/c. Some care must be taken in choosing values for μ and b which yield convergence in a reasonable time frame without overdamping the system. The binding energies of these ground states were found to be reproducible at the level of a few hundredths of an MeV per nucleon for different starting conditions.

The cpu time required to follow a ground state out to 200 fm/c varies like A^2: from less than 3 min for $A=50$ to about 40 min for a mass 200 isotope (times quoted for a single IBM 3081 processor). The long running times for heavy nuclei prevented us from doing a complete χ^2 minimization search. Instead, our attention was focused on the binding energies and rms radii of a few nuclei in the 40, 110, and 200 mass range. It was found that the parameter set $A=-129.69$, $B=74.24$, $C=30.54$ MeV, and $G=291$ MeV fm^5 produced acceptable ground states for these nuclei.

Several different means can be used to assess the quality of these ground states. We begin with a general sample of nuclei over the periodic chart, as shown in Table I. Looking first at the binding energies, one can see that the agreement between the model and the data is typically at the few tenths of an MeV per nucleon. Considering how few parameters are present in the model, this is about the level of agreement which one would expect. For example, the table also shows the fit obtained by Green[2] with a mass formula of a similar number of parameters, and one can see that the level of accuracy is comparable. Since our model is complete, we can also predict rms radii and a comparison between these predictions and those obtained in the Woods-Saxon fit[17]

$$\rho(r) = \rho_0\{\exp[(r-R)/a]+1\}^{-1} ,$$
$$a = 0.545 \text{ fm} , \tag{22}$$
$$R = 1.18A^{1/3} - 0.48 \text{ fm}$$

is also shown. Again, the predictions are remarkably close to the fits.

The isospin dependence of the binding energies is also reproduced fairly well as evidenced by the agreement found for heavy nuclei in Table I. This can be treated further by choosing an isobaric sequence, as is shown in Table II. In this table, two intermediate mass systems are chosen, $A=32$ and 51. Again, the agreement with experiment is very reasonable.

One of the problems which most classical models of

TABLE I. Model calculations of binding energies per nucleon and rms radii for selected nuclei. The predictions for the binding energies are compared with both the data and the mass formula of Green (Ref. 20). The rms radii are compared with that obtained in a Woods-Saxon fit to a range of nuclei.

Nucleus		Binding energy per nucleon (MeV)			rms radius (fm)	
A	Z	Model	Data	Green	Model	Woods-Saxon
10	5	6.77	6.48	6.67	2.47	2.58
20	10	7.34	8.03	7.89	2.80	2.96
40	20	8.19	8.55	8.47	3.27	3.42
52	24	8.75	8.78	8.74	3.41	3.65
58	28	8.60	8.73	8.65	3.57	3.76
88	38	8.80	8.73	8.69	4.03	4.21
108	47	8.70	8.54	8.57	4.27	4.47
197	79	8.07	7.92	7.90	5.17	5.35

TABLE II. Isospin dependence of binding energy per nucleon. The comparison is made between the model calculation, data, and a fit to the data.

Nucleus		Binding energy per nucleon (MeV)		
A	Z	Model	Data	Green
32	14	8.15	8.48	8.40
32	15	8.09	8.46	8.48
32	16	7.97	8.49	8.36
32	17	7.69	8.07	8.03
51	21	8.68	8.60	8.56
51	22	8.73	8.71	8.69
51	23	8.74	8.74	8.74
51	24	8.70	8.71	8.71
51	25	8.56	8.63	8.59

nuclei encounter is the description of light nuclei. The ground states of classical-point particles moving in Yukawa potentials are often overbound and/or have incorrect radii. The results obtained with this model should be better since (i) a density-dependent potential is used and the average density of the quasiparticle system will decrease with decreasing mass and (ii) a finite rms radius will be obtained even when the quasiparticles are coincident, because of their finite width.

The results for light nuclei are shown in Table III. Even the deuteron, which is difficult to handle classically because of its broad wave function, has approximately the correct characteristics. Further, we find that $A=5$ system are significantly less well bound (per nucleon) than ^{4}He. Unfortunately, the energetics are not quite correct and certain $A=5$ systems remain particle stable, just as does ^{8}Be. The rest of the light nuclei have binding energies and rms radii which are close to their observed values.

We find, then, that the binding energies and radii predicted by this model are in quantitative agreement with experiment at the tenths of an MeV per nucleon level over the entire periodic chart. Further, the accuracy of the masses generated in this dynamical model are competitive with those obtained in a simple parametrized mass formula fitted to the data. This is not to suggest that the model should be used in place of a mass formula for predicting ground-state properties (if for no other reason than the computer time required to obtain an answer). However, the model does possess the accuracy required for comparison with experiment for measurements sensitive to the properties of nuclei at low excitation energies.

TABLE III. Binding energies and rms radii for light nuclei. The comparisons are the same as Table I.

Nucleus		Binding energy per nucleon (MeV)			rms radius (fm)
A	Z	Model	Data	Green	Model
2	1	2.71	1.11	1.34	2.45
3	1	4.37	2.83	0.61	2.45
4	2	6.24	7.07	4.09	2.45
5	2	5.84	5.48	4.06	2.48
6	3	6.06	5.33	5.37	2.45
7	3	6.52	5.61	5.49	2.45
8	4	7.09	7.06	6.14	2.45
9	4	6.88	6.46	6.29	2.47
10	5	6.77	6.48	6.67	2.47
12	6	6.97	7.68	7.05	2.55

In applying the model to heavy-ion collisions, as will be done in the next paper of this series, there may be some observables which are sensitive to the slight inaccuracies in the binding energies predicted for the light systems. However, the predictions can be made more accurate by the use of an afterburner code to allow for the decays of particle unbound states. In such a procedure, the excitation energies of the predicted products of the collision are determined by comparing the binding energies of the products with the ground-state energies of the computational nuclei. A statistical decay code based on the observed masses is then used to follow the decays. The only time-consuming step in this procedure is the initial generation of the ground-state energies of the computational nuclei over the mass range of interest. Thus far, we have calculated the binding energies of all nuclei within ± 7 charge units of the locus of the most stable nuclei up to $A=110$.

V. CONCLUSION

We have formulated a computational model for nuclear dynamics studies based on the following considerations: (i) the execution time to evaluate the forces or energy in an N-nucleon system must scale only as βN^2, where β must be small; (ii) the ground states must possess a finite value for $\langle p^2 \rangle$; (iii) the computational ground states must be the true ground states of the interaction used (unlike Refs. 5–7, which use metastable states) and possess binding energies and radii which are close to the observed values over a broad mass range.

The first criterion led us to avoid test-particle methods [which scale like $\beta(tN)^2$, where t is the number of test particles per nucleon] and towards the use of a momentum-dependent two-body potential to represent antisymmetrization effects. The potential which was obtained not only satisfied criterion (ii), but also possessed a value of the energy distribution which is close to that of a fermion system in the absence of other interactions.

A simple form was chosen for the nuclear potential energy density, and it was shown that this form led to binding energies and radii which were quantitatively comparable with experiment (at the 90% level of accuracy or better) over the entire periodic chart. Further, the interaction also possessed the commonly accepted properties of nuclear matter. Of course, there are many other nuclear interactions available than the one we have used: Ours was chosen solely for its simple functional form and small number of parameters.

The advantages of using this approach in the study of fragmentation include the following: Here, the cold nuclei are true classical ground states of a Hamiltonian, and these ground states are straightforward to determine. In turn, this means that the excitation energy of reaction

products can be computed.

However, the model is still only an approximation to the real quantum many-body theory, and there are a number of features which it lacks. First, this Pauli potential shares with others previously proposed the problem of inducing a scattering phase shift between like particles at low energies, although this problem is not particularly important in nuclear reactions. As well, the width of the wave packets is fixed in this model, whereas it should be allowed to evolve with time. This last difficulty could be partly solved with the inclusion of an equation of motion for the width α, or (at a substantial increase in computer time requirements) through the use of test particles.

ACKNOWLEDGMENTS

The authors wish to thank G. Bertsch (Michigan State University) for stimulating their interest in this problem and providing useful criticisms of the manuscript. We also wish to thank J. Randrup (Lawrence Berkeley Laboratory) and G. Fai (Kent State University) for useful discussions. One of us (D.H.B.) would like to acknowledge the support of Lawrence Livermore Laboratory and Lawrence Berkeley Laboratory for their hospitality while this project was in progress. This work was supported in part by the Natural Sciences and Engineering Research Council of Canada.

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