

Exact calculations of the ground state of model neutron matter*

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We report results of Monte Carlo variational calculations for a simple model of neutron matter for three different internuclear potentials. We have also done exact Monte Carlo calculations for the ground state of one of these systems. A wave function for the solid phase with full symmetry is proposed. None of the three systems crystallize. The validity of the Wu-Feynberg expansion and hard-sphere modeling for these systems are discussed.

I. INTRODUCTION

Because of the interest in the interior of pulsars, dense neutron matter has been studied theoretically by a variety of approximation techniques. The review article by Baym and Pethick gives the background and references on this problem.¹ Because of the complexity of the neutron interaction, most authors have chosen a simple model for it, solved the many-body problem approximately, and thereby obtained the equation of state and the solidification density (if any). Among the approximations used have been a generalization of the law of corresponding states,^{2,3} a hard-sphere model,⁴ and a constrained variational method based on the hypernetted-chain equation.⁵ In order to decide which approximations are accurate for this very soft but short-range potential, we have performed an essentially exact numerical calculation for a system of Bose particles interacting with a repulsive Yukawa potential, and the computations have been carried out for a wide range of densities.

Our model of nuclear matter is a system of bosons with the following Hamiltonian:

$$H = \sum_{i=1} \frac{P_i^2}{2m} + \sum_{i < j} \epsilon \frac{\exp(-r_{ij}/\sigma)}{r_{ij}}. \quad (1)$$

The values of ϵ and σ were chosen to agree with previous work; for the Cochran-Chester⁶ (CC) potential, $\epsilon = 5725$ MeV fm and $\sigma^{-1} = 4.1$ /fm, and for the "homework" (HW) potential,⁷⁻¹⁰ $\epsilon = 9263.14$ MeV fm and $\sigma^{-1} = 4.9$ /fm. One can characterize a Yukawa potential by the dimensionless quantum parameter Λ^* , just as is done with stiff-core systems, where

$$\Lambda^* = \frac{\hbar}{\sigma \sqrt{m \epsilon}}.$$

This quantum parameter changes little from the

CC to the HW potential (1.08 to 0.93). We expect, therefore, to find little difference in the physical properties of systems with these values of Λ^* . We should also mention that the Yukawa potential is of considerable interest in itself because it is a radically different potential as compared with either the Coulomb potential (long range and soft) or the hard-core potentials (short range and stiff). The short range and the soft character of this potential may well lead, quite generally, to different physical behavior. For densities significantly above nuclear-matter density ($\rho = 0.17$ fm⁻³), a nonrelativistic Hamiltonian does a very poor job of representing real neutron matter. There are, however, three reasons for using such a simple Yukawa model. First, various approximate methods have been tried out on this potential, where the physics is rather simple. The main complication is the many-body nature of the ground state. If the approximate methods work well with this Hamiltonian there is a good chance they will also do well for a more realistic Hamiltonian. Second, exact methods exist for computing the ground-state properties of this Hamiltonian that have worked well for the hard-sphere boson system. In order to use this method for a relativistic neutron potential many extensions of the present method would have to be invented. Third, such a potential is a screened Coulomb potential, and for sufficiently high densities ($\sigma \rho^{-1/3} \ll 1$) the system should behave as a quantum one-component plasma with

$$r_s = \frac{m}{\hbar^2} \epsilon \left(\frac{3}{4\pi \rho} \right)^{1/3}. \quad (2)$$

II. THE METHOD OF CALCULATION

A. Variational calculations

Our calculations have two steps. First, a good variational or trial wave function Ψ_J is found, and

TABLE I. The potential is given by Eq. (1) and Eq. (18); ρ is the density in fm^{-3} ; A , B , and D are the variational parameters [see Eq. (4)]; E , T , and E_{static} (Madelung) are the variational energy, kinetic energy, and static or classical energy in MeV. $\Delta E_{\mathcal{F}}$ is the first term of the Wu-Feenberg expansion, and N_0 is the variational condensate fraction. The figures in parentheses in the column labeled E show the errors in the quoted energies.

Potential	ρ	A	B	D	E	T	E_{static}	$\Delta E_{\mathcal{F}}$	N_0
CC	0.2	2.1	0.9	0.25	100.4(0.4)	38.1	8.45	19.6	0.57
CC	0.5	2.2	0.9	0.25	347.0(1.0)	101.7	89.5	23.8	0.41
CC	1.0	2.2	1.7	0.20	883.0(3.0)	160.0	380.8	7.5	0.40
CC	5.0	1.9	2.6	0.18	7 113.0(9.0)	517.0	5302.	-105.8	0.28
CC	10.0	1.5	3.4	0.14	16 273.0(12.0)	1059.0	13 484.	-336.3	0.26
HW	0.3	2.8	1.0	0.40	137.6(0.7)	61.0	9.09	28.5	0.47
HW	1.0	3.0	1.5	0.20	725.6(1.3)	260.0	214.5	32.9	0.24
HW	2.0	2.5	2.1	0.19	1 857.0(5.0)	351.0	886.1	-21.4	0.28
Schiff	1.34	2.5	2.0	0.30	262.0(3)	205.0	-253.7	53.9	0.40
Schiff	1.96	2.3	2.2	0.30	524.0(6)	259.0	-246.7	38.9	0.38
Schiff	2.80	2.15	2.5	0.25	969.0(7)	361.0	-117.6	14.6	0.36

second, it is used to importance-sample the random walk in the exact calculation. The accuracy of the ground-state energy and the amount of computer time needed for convergence to the ground state are directly related to how good the trial wave function is. For this problem a modification of the Cochran-Chester⁶ wave function (of the Jastrow type) is a very good approximation to the ground state:

$$\Psi_J(R) = \prod_{i < j} e^{-u(r_{ij})} \prod_k e^{-\chi(r_k)}, \quad (3)$$

where

$$u(r) = \frac{Ae^{-Br}}{\gamma} (1 - e^{-r/D}). \quad (4)$$

The pseudopotential $u(r)$ reduces to that of Cochran and Chester for $D=0$; with $D \neq 0$ it allows for s -wave penetration of the ground state.¹¹

The square of this wave function was sampled using standard Monte Carlo techniques¹² to evaluate the integrals which arise in the expectation value of the Hamiltonian, a method that has been well tested on other boson systems.¹³ The density range extended from a typical nuclear-matter density to 50 times that. For all but the highest densities 54 particles were found to be sufficient to represent the bulk properties. Table I shows the results of these calculations, some of which were obtained by Cochran.⁶

In order to calculate the difference in energy between expectation values computed from two nearby Jastrow functions, the technique of correlated sampling was used. Configurations from one variational calculation were saved, and later the difference in energy for a change in Jastrow parameters was calculated by weighting the energy estimator by the ratio of the square of the new

Jastrow function to that of the old. Theoretically one could find the energy for *any* set of Jastrow parameters and thus determine the optimum set of parameters at once. But for the results to be reliable the weights must be of the same order of magnitude, and this limits one to choosing the new Jastrow parameters in the neighborhood of the old ones. However, this technique does allow one to determine the optimum wave function more quickly and with more precision than a simple variational search, because the variance of the energy difference is much smaller than would be obtained by independent runs.

The function χ is a single-particle function which localizes the particles on lattice sites and hence describes a solid. The usual choice is a Gaussian wave function¹⁴

$$\chi_G(\vec{r}) = C(\vec{r} - \vec{R}_j)^2, \quad (5)$$

where \vec{R}_j is a lattice site and C is a variational parameter. With this choice of χ_G the many-body wave function is not symmetric with respect to particle interchange. If a crystal state exists for this repulsive Yukawa potential, it is not unlikely that the particles will be only weakly tied to their lattice sites, and exchange effects could be important. Also if particles are not well localized in the true ground state we must use a symmetric trial wave function in the exact method to importance-sample the random walk; otherwise such exchange effects could be exceedingly rare and the convergence exceedingly slow. The simplest function which has all the proper symmetries for a bcc lattice (except invariance under translation) is

$$\chi_E = (C/k^2)(\cos kx \cos ky + \cos kx \cos kz + \cos ky \cos kz), \quad (6)$$

where $k = 2\pi/a$ and $a =$ lattice spacing. This is normalized to have the same curvature at a lattice point as χ_G , and will therefore behave the same as χ_G for a well-localized bcc crystal (large C). The main disadvantage with this wave function is that the barriers between lattice points are not as steep as for the Gaussian wave function, and thus it does not keep the particles as well separated. In the random walk required by the method of Metropolis *et al.*¹² considerable "diffusion" through the lattice occurs. One could, of course, add in more symmetrized combinations of plane waves but that complicates the variational search, and the exact method does not need them.

Our variational computations for both the CC and HW potentials show that the many-body wave function constructed from χ_E has a lower energy than that constructed from χ_G for all values of C . The energy increases monotonically with respect to C from the liquid values.¹⁵ This monotonic increase has been independently verified by calculating the derivative of the energy with respect to C using the reweighting procedure described above. Thus the Monte Carlo calculations show that χ_E is at least as good a wave function as χ_G , and that for these two potentials the liquid has a lower energy than the solid for all densities. For high densities this system approaches the quantum one-component plasma. Pollack and Hansen have published an estimate of the solid-liquid transition density.¹⁶ Since the highest density we have studied is considerably higher than that density,¹⁷ we conclude on the basis of their estimate that the boson ground state for either potential (CC or HW) will not crystallize at any density.

B. Exact computations

The method for finding the exact ground-state wave function is a version of a Monte Carlo Green's-function algorithm developed and used by Kalos *et al.*^{18,19} for the hard-sphere ground state. Let \vec{R}_0 be a $3N$ -dimensional coordinate, where N is the number of particles. The algorithm finds a new coordinate \vec{R} with the probability density given by $\tilde{G}(\vec{R}, \vec{R}_0)$, where

$$\tilde{G}(\vec{R}, \vec{R}_0) = E_t \frac{\Psi_J(\vec{R})}{\Psi_J(\vec{R}_0)} G(\vec{R}, \vec{R}_0), \quad (7)$$

and $G(\vec{R}, \vec{R}_0)$ is the Green's function for the Hamiltonian [Eq. (1)]

$$H(\vec{R})G(\vec{R}, \vec{R}_0) = \delta^{3N}(\vec{R} - \vec{R}_0). \quad (8)$$

Initial coordinates \vec{R}_0 are drawn from $\Psi_J^2(\vec{R}_0)$, the function found from the variational calculation. A new generation of points is constructed by sampling $\tilde{G}(\vec{R}, \vec{R}_0)$. If $\Psi_{n-1}(\vec{R}_0)\Psi_J(\vec{R}_0)$ is one generation,

the next generation has a density function

$$\Psi_n(\vec{R})\Psi_J(\vec{R}) = \int d\vec{R}_0 \tilde{G}(\vec{R}, \vec{R}_0) \Psi_{n-1}(\vec{R}_0) \Psi_J(\vec{R}_0). \quad (9)$$

The process of constructing a new generation of points is repeated until all the available averages above have converged. It is easy to see that the final configurations will be drawn from $\varphi_0(\vec{R})\Psi_J(\vec{R})$, where $\varphi_0(\vec{R})$ is the ground state. The Green's function can be expanded in terms of the eigenfunctions of the Hamiltonian H ; $\varphi_\alpha(\vec{R})$. Thus

$$G(\vec{R}, \vec{R}_0) = \sum_\alpha \frac{\varphi_\alpha(\vec{R})\varphi_\alpha(\vec{R}_0)}{E_\alpha} \quad (10)$$

and

$$\Psi_J(\vec{R}_0) = \sum_\alpha C_\alpha \varphi_\alpha(\vec{R}_0).$$

Then,

$$\Psi_n = \sum_\alpha C_\alpha \left(\frac{E_t}{E_\alpha}\right)^n \varphi_\alpha(\vec{R}). \quad (11)$$

If E_t is adjusted so that the number of output configurations is about the same as the number of input configurations, then the configurations should converge exponentially to the ground state. Typically 40 to 100 iterations of Eq. (9) are necessary to reach the ground state for this system.

Two different estimators are used to find the ground-state energy. The first is the eigenvalue of Eq. (9), or the ratio of the number of elements in successive generations:

$$E_G = E_t \int d\vec{R} \Psi_n(\vec{R})\Psi_J(\vec{R}) / \int d\vec{R} \Psi_{n+1}(\vec{R})\Psi_J(\vec{R}). \quad (12)$$

The second is the variational energy:

$$E_J = \int d\vec{R} \Psi_n(\vec{R}) H \Psi_J(\vec{R}) / \int d\vec{R} \Psi_n(\vec{R}) \Psi_J(\vec{R}), \quad (13)$$

where E_J is the ground-state energy since H is Hermitian. Elsewhere we will publish more details of the exact method including refinements which increase the accuracy considerably.

A number of different checks of the method were used. To be sure of convergence the program was run many generations beyond the point at which E_G appeared constant. The two independent estimators of the energy gave the same value within statistical errors although the second, Eq. (13), had somewhat less variance. The size of the system was increased from 54 to 128 particles, and the small shift in energy was the same as in the variational calculation. A bad trial function, one that was deliberately less restrictive and whose variational energy was 20% higher, was used. The

final answers should be insensitive to this change. As expected, the variance of the energy and the convergence time increased, but the ground-state energy remained the same within statistical errors.

These tests indicate that the results are reliable. In Table II the final energies are shown. The quantities denoted in the table as "mixed" come from an average over $\Psi_n \Psi_J$. For example, if $V(\vec{R})$ is the potential energy of the system the variational potential energy is

$$V_{\text{var}} = \int d\vec{R} V(\vec{R}) \bar{\Psi}_J^2(\vec{R}) / \int d\vec{R} \bar{\Psi}_J^2(\vec{R}). \quad (14)$$

The exact potential energy is

$$V_{\text{ex}} = \int d\vec{R} \varphi_0^2(\vec{R}) V(\vec{R}) / \int d\vec{R} \varphi_0^2(\vec{R}), \quad (15)$$

and the "mixed" potential energy is

$$V_{\text{mix}} = \int d\vec{R} V(\vec{R}) \varphi_0(\vec{R}) \bar{\Psi}_J(\vec{R}) / \int d\vec{R} \varphi_0(\vec{R}) \bar{\Psi}_J(\vec{R}). \quad (16)$$

If the trial wave function is close to the ground state, the mixed results are the arithmetic means of the exact values and the variational values.²⁰ Another calculation involving more iterations can be done if one wants to find the exact ground-state values of quantities other than the energy, for example, the two-particle correlation function, the kinetic energy, the potential energy, or the single-particle density matrix.²¹

The single-particle density matrix was computed by the method of McMillan.¹³ The variational and mixed results are shown for the condensate fraction in the zero-momentum state. An improvement of the method described by Kalos²¹ was employed to determine this fraction exactly at one density. It is difficult to make a direct comparison of the condensate fractions found in this sys-

tem with those found in hard-core systems.¹⁴ This is simply because the potentials are fundamentally different. If we take $n\sigma^3$ as the natural way in which to measure the density for both types of systems (Yukawa and hard core), then the following rough comparison can be made; for the CC potential the condensate fraction is 33% when $n\sigma^3 = 0.15$, and for the hard-core potential the condensate fraction is 10% when $n\sigma^3 = 0.20$. This suggests that there is much freedom of movement in the ground state and the system is probably more of a gas than a dense liquid.

The variational energies are less than 1% above the exact results. The variances in the energies are also much smaller than in a hard-sphere calculation for a comparable computing time. Clearly the Jastrow function is a very good approximation to the ground state for this soft-core potential. The Jastrow function is not as good for estimating other quantities, as evidenced by the differences between the variational and mixed results. The mixed two-particle correlation function $g(r)$ is also very close to the variational $g(r)$ with the mixed g showing about 5% more structure than the other.

Several papers have used the Wu-Feenberg expansion approximately to antisymmetrize the wave function.^{4,22} The first term of this expansion, including the ideal Fermi gas energy, is shown in Table I. For the higher densities it becomes negative. The sum of the whole series is positive since Fermi statistics must raise the energy. This can easily be shown with the aid of the Feynman theorem.²³ If Ψ_B and E_B are the ground-state wave function and the ground-state energy of the Bose system, and $F\Psi_B$ and E_F are the corresponding fermion quantities then

$$E_F = E_B + \frac{\hbar^2}{2m} \int d\vec{R} \bar{\Psi}_B^2 |\vec{\nabla} F|^2 / \int d\vec{R} |F\Psi_B|^2. \quad (17)$$

Since the second term on the right-hand side is positive, $E_F \geq E_B$. If the first term of the series is negative it is unlikely that the first two terms of the Wu-Feenberg expansion will be accurate enough to compute the difference between the liquid and solid phases, particularly since the convergence of the series is likely to be different in the two phases. Later we will publish the results of a variational study and an exact study, in which we use a fully antisymmetric wave function with the nodes of the ideal-Fermi-gas wave function.

Schiff⁴ has used a quantum perturbation technique to calculate the equation of state of neutron matter from the equation of state of hard-sphere

TABLE II. The potential is the CC potential of Eq. (1); ρ is the density in fm^{-3} , and E_0 is the exact ground-state energy in MeV. The figures in parentheses in the column labeled E show the errors in the quoted energies. T_{mix} and $N_{0\text{mix}}$ are the kinetic energy and the condensate fraction calculated from the function $\varphi_0(R)\Psi_J(R)$. $N_{0\text{ex}}$ is the exact value of the condensate fraction (for all but $\rho = 1$ this is extrapolated from the variational and mixed results).²⁰

ρ	E_0	T_{mix}	$N_{0\text{mix}}$	$N_{0\text{ex}}$
0.2	99.7 (0.6)	38.9	0.56	0.57
0.5	341.0 (0.4)	102.5	0.41	0.40
1.0	880.0 (2.0)	170.0	0.38	0.38
10.0	16 248 (14)	1039.0	0.29	0.33

bosons. The potential he chooses for the neutron interaction has the repulsive part of the Reid potential with half of the attractive part;

$$V(r) = (C_1 e^{-x} + C_2 e^{-4x} + C_3 e^{-7x})/x, \quad x = (0.7 \text{ fm}^{-1})r,$$

where

$$C_1 = -5.261 \text{ MeV},$$

$$C_2 = -825.8 \text{ MeV},$$

$$C_3 = 6484.2 \text{ MeV}.$$

At high densities an attractive potential will undergo total collapse if the core is not sufficiently repulsive relative to the depth of the attractive well (e.g. the soft-core Reid 1S_0 potential). On the other hand, if the core is sufficiently repulsive it will behave like a repulsive Yukawa potential, and we can make a correspondence by requiring that the potentials have the same behavior at small r . In particular, the effective Yukawa parameters ϵ and σ [see Eq. (1)] can be found by requiring that the two potentials have the same terms in r^{-1} and r . With this requirement the Schiff potential has an effective $\epsilon = 8076 \text{ MeV fm}$, $\sigma^{-1} = 5.14 \text{ fm}^{-1}$, and $\Lambda^* = 1.02$. This argument suggests that the Cochran-Chester wave function will be good at high densities, and that the equation of state for Schiff's potential will be close to that of this potential.

We have calculated the energy of this system variationally using the wave function in Eq. (3) for the same density range as Schiff. We find that his model seriously overestimates the energy and pressure (see Table I and Fig. 1). This increase occurs because the kinetic energy in his model is the kinetic energy of a system of hard-sphere bosons (with a radius of 0.25 fm), and this increases very rapidly with increasing density. The hard spheres must avoid close approaches because the wave function must vanish when two particles touch; this gives the wave function a large curvature at high densities. But for a soft-core potential the wave function no longer has to vanish, and there is therefore much more "available space" between the particles so the wave function can spread out and lower its curvature.

Another approximation scheme, constrained variation,⁵ where the many-body Schrödinger equation is replaced by a two-body equation with boundary conditions appropriate to a fluid, seems to work fairly well. The simplest approximation of this sort, the lowest-order constrained variation, gives energies about 20% higher than our variational results for both CC and HW potentials.²⁴ A slightly more complicated method based on the hypernetted-chain approximation for a fluid agrees with our result to within approxi-

mately 5%.⁵ These approximations will be fairly reliable as long as the system resembles a gas and exhibits no strong correlations. However, they probably are not accurate for estimating the liquid-solid phase transition since for soft-core potentials very small differences in energy may be important.¹⁶

In conclusion we find three significant differences between the ground state of a hard-core quantum liquid and a soft-core quantum liquid. For a soft core the Jastrow, or product-type, wave function appears to be an excellent approximation to the ground state for the purpose of computing the energy. An integral equation technique, based on the hypernetted chain equation, also gives rather accurate energies for this system. For soft cores, the particles can move about much more freely, and for this reason particle exchange in the solid is likely to be an important effect near any solid-liquid phase transition.

In contrast to the hard-core system, the Wu-

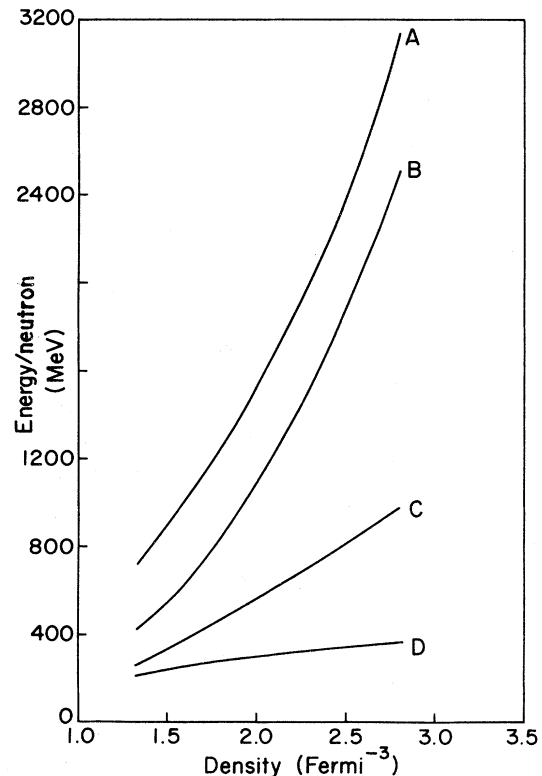


FIG. 1. Energy per neutron versus density for the attractive potential of Eq. (18). *A* is the kinetic energy of a hard-sphere liquid with a sphere diameter of 0.5 fm. *B* is the total energy per neutron as calculated by Schiff using a hard-sphere model. *C* and *D* are, respectively, the kinetic energy and the total energy of this system computed variationally using the wave function of Eq. (3).

Feenberg expansion is not a quickly convergent series and an accurate treatment of a completely antisymmetric wave function must be used. Finally, as Cochran and Chester point out,⁶ a soft-core

potential cannot be treated as a perturbation from a hard-core potential. It is likely that any treatment which relies on a correspondence between hard-core and soft-core systems will fail.

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¹⁵That is, no metastable solid state exists for these potentials. The metastability that Cochran found was apparently either a statistical fluctuation or an artifact of his wave function.

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²⁰Let $\delta = \Psi_j - \varphi_0$, and expand Eqs. (14) and (16) in terms of this difference, dropping all higher-order terms. We have checked this rule by changing the Jastrow function and observing that the projected exact value $V_{\text{ex}} = 2V_{\text{ini}} - V_{\text{var}}$ remained fixed within errors.

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